STRUCTURE OF A COMPLEX OF RETINOBLASTOMA PROTEIN BOUND TO E2F, AND USES THEREOF

The present invention relates to the crystal structure of pRb/E2F$_{(409-426)}$ as well as uses of the structure in identifying agents which modulate the binding between pRb and E2F and/or a pRb/E2F$_{(409-426)}$ complex, and thus are useful as pharmaceutical agents in the prevention or treatment of proliferative diseases.

The retinoblastoma tumour suppressor protein (pRb) regulates the cell cycle, sponsors differentiation and restrains apoptosis. Dysfunctional pRb is thought to be necessary for the development of most human malignancies.

pRb controls the cell cycle and apoptosis by acting as a negative regulator of transcription. It is now established that the growth-inhibitory effects of pRb are dependent on its regulation of the E2F family of transcription factors whose activity is necessary for the expression of genes involved in the G1 to S transition of the cell cycle and DNA replication. The transcriptional repression exerted by pRb over E2F responsive promoters involves at least three, distinct mechanisms. By binding to the transcriptional activation domain of E2F, pRb prevents it from recruiting components of the transcriptional apparatus and, once tethered to E2F promoters, pRb interacts with, and represses, other nearby transcription factors. Finally, pRb recruits protein factors to E2F promoters, such as histone deacetylases (HDACs) and histone methyltransferases (HMTases) that negatively regulate transcription by altering chromatin structure.

In addition to regulating entry into S-phase, it is thought that pRb is important in protecting differentiating cells from apoptosis. Certainly in many types of tissue, loss of pRb leads to apoptosis. This and other data has led to a model whereby the anti-apoptotic activity of pRb is mediated by its repression of certain E2F-dependent promoters. Unrepressed E2F is able to drive apoptosis by both p53-dependent and p53-independent mechanisms.

Although inactivation of the pRb pathway is thought to be widely involved in cellular transformation, there are examples of tumours where over-expression of functional pRb appears to be detrimental to successful clinical treatment. For example, adenocarcinoma of the pancreas is the fifth most common cause of cancer-related death in the Western world. It is particularly resistant to currently available forms of chemotherapy and radiation therapy. It is thought that this malignancy is able to evade apoptosis induced by treatment with chemotherapeutic drugs because of over-expression of pRb. It seems plausible that the protective effect of pRb over-expression against apoptosis is mediated by E2F. By blocking transcriptional activation by E2F, over-expression of pRb appears to render pancreatic cancer cells insensitive to chemotherapy.

As many of the anti-tumourigenic properties of pRb are mediated by its regulation of the E2F transcription factors, it would be beneficial to have a crystal structure of the pRb-binding fragment of E2F ($E2F_{(409-426)}$) in complex with the tumour suppressor protein. Such detailed knowledge of the molecular interactions between E2F and the A/B interface of pRb would enable the development of compounds that bind to pRb and inhibit complex formation. Such a compound, administered in parallel with conventional chemotherapy, would offer a means of enhancing treatment of proliferative diseases such as pancreatic cancer and perhaps related diseases.

Accordingly, the present invention provides the crystal structure of the primary pRb-binding fragment of E2F ($E2F_{(409-426)}$) in complex with the tumour suppressor protein pRb. The structure shows how $E2F_{(409-426)}$ binds at the interface of the A and B domains of the pocket of pRb making extensive interactions with conserved residues from both.

In order to address the regulation of the E2F transcription factor by pRb, the present inventors have determined the crystal structure of the complex of pRb_{AB} bound to the

minimal binding region of E2F, namely $E2F_{(409-426)}$. The structure has important implications for the understanding of pRb/E2F function. The studies have quantified the contribution of the principal interaction made by E2F through residues 409-426 with pRb as well as that of a secondary interaction involving the marked box region of E2F. In both cases these interactions are with the pocket region of the tumour suppressor protein pRb.

The analysis of the crystal structure of pRb/$E2F_{(409-426)}$ suggests that $E2F_{(409-426)}$ acts as a sensor of the structural integrity of the pRb pocket. Accordingly, cells in many tissues should be protected against deleterious mutations in pRb because they will sponsor increased E2F transcriptional activation, and thus apoptosis. It seems particularly intriguing, therefore, that all tumour derived pRb mutants fail to bind to E2F suggesting that an intense selectionary pressure operates in many types of tissue in favour of cells which harbour defects in apoptosis once they have lost normal pRb function. Perhaps the most notable exception to this process occurs in retinal cells, which are able to survive for some time with loss of pRb without acquiring other genetic alterations. Indeed, it has been suggested that these particular cells are distinguished by their ability to acquire survival signals from neighbouring cells and thus give rise to the eponymous retinoblastomas.

According to a first aspect, the present invention provides a crystal structure of the pRb/$E2F_{(409-426)}$ complex, characterised by the atomic co-ordinates of Annex 1.

Preferably the interactions between $E2F_{(409-426)}$ and pRb comprise one or more of the following interactions:

$E2F_{(409-426)}$ residue	**pRb residue**
Leu_{409}	Lys_{548}
Tyr_{411}	Glu_{551}

$E2F_{(409-426)}$ residue	pRb residue
Tyr_{411}	Ile_{532}
Tyr_{411}	Glu_{554}
His_{412}	Arg_{656}
His_{412}	Lys_{653}
Gly_{414}	Glu_{533}
Gly_{414}	Lys_{652}
Leu_{415}	Leu_{649}
Leu_{415}	Glu_{553}
Leu_{415}	Lys_{537}
Glu_{417}	Lys_{537}
Gly_{418}	Arg_{467}
Glu_{419}	Thr_{645}
Arg_{422}	Glu_{464}
Asp_{423}	Arg_{467}
Leu_{424}	Lys_{530}
Phe_{425}	Phe_{482}
Phe_{425}	Lys_{475}

In a second aspect, the present invention provides a method to identify an agent which modulates the interaction between pRb and $E2F_{(409-426)}$, the method comprising:-

a) combining together pRb, $E2F_{(409-426)}$ and an agent, under conditions in which pRb and $E2F_{(409-426)}$ form a complex;

b) growing a crystal of any pRb/$E2F_{(409-426)}$ complex; and

c) analysing the crystal structure to determine whether the agent is an agent which modulates the interaction between pRb and $E2F_{(409-426)}$.

In the present invention, the term "modulates" is intended to refer to inhibiting, enhancing, destabilising and/or stabilising the interaction between pRb and $E2F_{(409-426)}$ and/or the formation of the pRb/$E2F_{(409-426)}$ complex and/or the stability of the complex after formation.

"conditions in which pRb and $E2F_{(409-426)}$ can form a complex" are those conditions in which pRb and $E2F_{(409-426)}$ form a complex in the absence of an agent. Therefore the effect of the agent on the interaction between pRb and $E2F_{(409-426)}$ and complex formation can be assessed.

Growing a crystal of a pRb/$E2F_{(409-426)}$ complex in step b) can be performed using methods well known to the person skilled in the art, for example using methods described in Practical Protein Crystallography 1999, McRee, D. E., Academic Press, San Diego, Ca, USA; and also in Protein Crystallization Techniques, Strategies and Tips 1999, Bergfors, T. M., International University Line, Ca, USA.

In the method, the combining of the pRb, $E2F_{(409-426)}$ and agent may be in any order. The order may be combining pRb with the agent and then adding the $E2F_{(409-426)}$. Alternatively, the order may be combining $E2F_{(409-426)}$ with the agent and then adding pRb, or combining pRb with $E2F_{(409-426)}$ and then the agent. For example, the pRb may be combined with $E2F_{(409-426)}$ before soaking the complex in the agent, preferably in a solution of the agent. In this regard, two of the pRb, $E2F_{(409-426)}$ and agent may be co-crystalised before adding the pRb, $E2F_{(409-426)}$ or agent, as appropriate.

Preferably step c) comprises comparing the crystal structure to the crystal structure of the first aspect of the invention.

The agent may be selected using the three dimensional atomic co-ordinates of Annex 1.

In a third aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising selecting an agent using the three-dimensional atomic coordinates of Annex 1.

Preferably, said selection is performed in conjunction with computer modeling.

Preferably the method comprises the further steps of:

a) contacting the selected agent with pRb and E2F$_{(409-426)}$ under conditions in which pRb and E2F$_{(409-426)}$ can form a complex; and

b) measuring the binding affinity of pRb to E2F$_{(409-426)}$ in the presence of the agent and comparing the binding affinity to that of pRb to E2F$_{(409-426)}$ when in the absence of the agent, wherein an agent modulates a pRb/E2F$_{(409-426)}$ complex when there is a change in the binding affinity of pRb to E2F$_{(409-426)}$ when in the presence of the agent.

The method may further comprise:

a) growing a supplementary crystal from a solution containing pRb and E2F$_{(409-426)}$ and the selected agent where said agent changes the binding affinity of the pRb/E2F$_{(409-426)}$ complex under conditions in which pRb and E2F$_{(409-426)}$ can form a complex;

b) determining the three-dimensional atomic co-ordinates of the supplementary crystal by X-ray diffraction using molecular replacement analysis;

c) comparing the three dimensional atomic co-ordinates with those for the crystal structure as defined in the first aspect of the invention; and

d) selecting a second generation agent using the three-dimensional atomic coordinates determined for the supplementary crystal.

Preferably, said selection is performed in conjunction with computer modeling.

In a fourth aspect there is provided a method of identifying an agent that modulates a pRb/$E2F_{(409-426)}$ complex, comprising:

a) contacting a selected agent with pRb and $E2F_{(409-426)}$ under conditions in which pRb and $E2F_{(409-426)}$ can form a complex; and

b) measuring the binding affinity of pRb to $E2F_{(409-426)}$ in the presence of the agent and comparing the binding affinity to that of pRb to $E2F_{(409-426)}$ when in the absence of the agent, wherein an agent modulates a pRb/$E2F_{(409-426)}$ complex when there is a change in the binding affinity of pRb to $E2F_{(409-426)}$ when in the presence of the agent.

There is a "change in the binding affinity" when the binding affinity either decreases or increases when in the presence of the agent. If a decrease is observed, the agent may be inhibiting the complex. If an increase is observed, the agent may be enhancing the complex.

The method of the fourth aspect may further comprise:

a) growing a supplementary crystal from a solution containing pRb and $E2F_{(409-426)}$ and the selected agent where said agent changes the binding affinity of the pRb/$E2F_{(409-426)}$ complex under conditions in which pRb and $E2F_{(409-426)}$ can form a complex;

b) determining the three-dimensional atomic coordinates of the supplementary crystal by X-ray diffraction using molecular replacement analysis;

c) comparing the three dimensional atomic co-ordinates with those for the crystal structure defined in the first aspect of the invention; and

d) selecting a second generation agent using the three-dimensional atomic coordinates determined for the supplementary crystal

Preferably, said selection is performed in conjunction with computer modeling.

In a fifth aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;
b) co-crystalising pRb with the agent;
c) determining the three dimensional coordinates of the pRb-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

In a sixth aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;
b) crystalising pRb and soaking the agent into the crystal;
c) determining the three dimensional coordinates of the pRb-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

In a seventh aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;
b) co-crystalising pRb, E2F$_{(409-426)}$ and the agent;
c) determining the three dimensional coordinates of the pRb-E2F-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

In an eighth aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;

b) co-crystalising pRb and $E2F_{(409-426)}$ and soaking the agent into the crystal;
c) determining the three dimensional coordinates of the pRb-E2F-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

Preferably the agent in the fifth, sixth, seventh or eighth aspect is selected using the three dimensional atomic co-ordinates of Annex 1. Preferably the method of the fifth, sixth, seventh or eighth aspect further comprises selecting a second generation agent using the three dimensional atomic coordinates determined. The second generation agent is preferably selected using the three dimensional atomic coordinates of Annex 1. The selection may be performed in conjunction with computer modeling.

Preferably the selected agent and/or the second generation agent, in the second, third, fourth, fifth, sixth, seventh and/or eighth aspects mimics a structural feature of $E2F_{(409-426)}$ when said $E2F_{(409-426)}$ is bound to pRb.

Preferably soaking refers to the pRb/$E2F_{(409-426)}$ complex being transferred to a solution containing the selected agent.

The method as defined in the third aspect preferably comprises the further steps of:
a) contacting the selected agent with a pRb/$E2F_{(409-426)}$ complex; and
b) determining whether the agent affects the stability of the complex.

Preferably the determination is with fluorescence polarization.

In a ninth aspect, the present invention provides a method of identifying an agent that modulates a pRb/$E2F_{(409-426)}$ complex, comprising:
a) contacting a fluorescently tagged $E2F_{(409-426)}$ peptide (E2F-fluoropeptide) with pRb to allow pRb/E2F-fluoropeptide complex formation;

b) detecting the fluorescence polarization;
c) adding a selected agent; and
d) detecting the fluorescence polarization in the presence of the agent.

In a tenth aspect, the present invention provides a method of identifying an agent that modulates a pRb/$E2F_{(409-426)}$ complex, comprising;

a) contacting a fluorescently tagged $E2F_{(409-426)}$ peptide (E2F-fluoropeptide) with pRb to allow pRb/E2F-fluoropeptide complex formation;
b) detecting the fluorescence polarization;
c) contacting a selected agent with pRb and $E2F_{(409-426)}$ peptide (E2F-fluoropeptide) under conditions in which pRb and E2F-fluoropeptide can form a complex;
d) detecting the fluorescence polarization; and
e) comparing the fluorescence polarization detected in b) and d).

Preferably the fluorescently tagged E2F peptide is selected using the three dimensional atomic co-ordinates of Annex 1.

Preferably a decrease in fluorescence polarization in the presence of the agent indicates that the agent destabilises the complex.

The methods of the ninth or tenth aspects may comprise the further step of adding untagged $E2F_{(409-426)}$ and detecting fluorescence polarization.

Preferably if fluorescence polarization decreases , on addition of the untagged $E2F_{(409-426)}$, the agent does not stabilise the complex.

Preferably if there is no substantial change in fluorescence polarization, on addition of the untagged $E2F_{(409-426)}$, the agent stabilises the complex.

Preferably the method further comprises:

a) contacting a fluorescently tagged E7 peptide (E7-fluoropeptide) with pRb to allow pRb/E7-fluoropeptide complex formation;
b) detecting the fluorescence polarization;
c) adding an agent that modulates pRb/E2F$_{(409-426)}$ complex; and
d) detecting the fluorescence polarization in the presence of the agent.

Alternatively the method may further comprise:

a) contacting a fluorescently tagged E7 peptide (E7-fluoropeptide) with pRb to allow pRb/E7-fluoropeptide complex formation;
b) detecting the fluorescence polarization;
c) contacting an agent that modulates pRb/E2F$_{(409-426)}$ complex with pRb and E7-fluoropeptide under conditions in which pRb and E7-fluoropeptide can from a complex;
d) detecting the fluorescence polarization; and
e) comparing the fluorescence polarization detected in b) and d).

Preferably a decrease in fluorescence polarization indicates that the agent also inhibits E7 binding to pRb. Such agents can then be removed from the method because the agents are identified as non-specific inhibitors. This identification of non-specific inhibitors can dramatically reduce the workload downstream of the assay method, for example in biochemical assays, thereby accelerating the hit to lead discovery process.

In addition ANS (aniline naphthalene sulphonic acid) reagent may be used to detect hydrophobic surfaces on pRb which become exposed as it unfolds. The fluorescence of ANS is highly sensitive to its environment. In solution there is virtually no fluorescence, whereas when bound to protein, such as pRb, it fluoresces highly. Changes in protein structure can alter the fluorescent signal of bound ANS due to changes in its enviroment to water. Therefore changes in pRb structure can be detected on addition of ANS and the agent that modulates pRb/E2F$_{(409-426)}$ complex. If the fluorescent signal alters on addition of the agent, the agent may be affecting the pRb

structure. The use of ANS to monitor protein unfolding is known in the art (Semisotnov et al (1991) Biopolymers, 31(1), 119-128)

The binding affinities may be measured by isothermal titration calorimetry. Alternatively the binding affinities may be measured by Surface Plasmon Resonance (SPR).

In an eleventh aspect, the present invention provides an agent identified by a method according to the second, third, fourth, fifth, sixth, seventh, eighth, ninth and/or tenth aspects of the invention.

In a twelfth aspect, the present invention provides an agent, as set out according to the eleventh aspect of the invention, for use as an apoptosis promoting factor in the prevention or treatment of proliferative diseases.

Preferably the, or each selected agent is obtained from commercial sources or is synthesised. Preferably the agent is for use in preventing or treating cancer, which may be pancreatic cancer and related diseases.

In a thirteenth aspect, the present invention provides the use of an agent, which modulates a pRb/$E2F_{(409-426)}$ complex, identified by a method according to the second, third, fourth, fifth, sixth, seventh, eighth, ninth and/or tenth aspects of the present invention, in the manufacture of a medicament for the prevention or treatment of proliferative diseases.

The proliferative diseases may be cancer, preferably pancreatic cancer and related diseases.

In a fourteenth aspect, the present invention provides the use of the atomic co-ordinates of the crystal structure as set out according to the first aspect of the present invention, for identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex.

In a fifteenth aspect, the present invention provides computer readable media comprising a data storage material encoded with computer readable data, wherein said computer readable data comprises a set of atomic co-ordinates of the pRb/E2F$_{(409-426)}$ crystal structure according to Annex 1 recorded thereon.

Preferred features of each aspect of the invention are as for each of the other aspects *mutatis mutandis*.

The present invention will now be described, by way of example only, and with reference to the following figures, in which:

Annex I.

Atomic co-ordinates for crystal of pRb/E2F$_{(409-426)}$ complex.

In Annex 1 there is shown:

Column Number	*Description*
2	Atom number
3	Atom type
4	Residue type
5	pRb domains (A or B) or E2F$_{(409-426)}$ (P)
6	Residue number
7	x co-ordinate of atom (Å)
8	y co-ordinate of atom (Å)
9	z co-ordinate of atom (Å)
10	Occupancy
11	B-factor (Å^2)

Figure 1.

Structure of pRb/E2F.

(A) Schematic drawing of functional domains and protein constructs used for pRb, E2F. The shading used for the constructs in this panel match those used in subsequent figures.

(B) The structure of $pRb_{AB}/E2F_{(409-426)}$, shown in two orthogonal views in Ribbons representation. The helices of the A domain are shown as a darker shade to those of the B domain. The main-chain trace of E2F is labelled.

(C) The interactions between $E2F_{(409-426)}$ and pRb_{AB} are shown schematically with the E2F peptide running down the centre. Residues of E2F that are conserved across the five family members are shown as ovals, while the five residue subset of these conserved residues whose mutation leads to disruption of the pRb/E2F interaction are shaded. Hydrogen-bond interactions are shown as broken lines, while hydrophobic contacts are indicated by bands. Residues from domain A of pRb are labelled with an asterisk and the other residues are from domain B. All of the pRb residues shown are either invariant or conserved across 27 species of pRb, p107 and p130.

Figure 2.

Isothermal Titration Calorimetry (ITC) measurements.

(A) The upper panel shows the raw data of an ITC experiment performed at 22°C. The lower panel shows the integrated heat changes, corrected for the heat of dilution, and the fitted curve based on a single site model. The panel represents the experiment where $E2F_{(243-437)}$ is titrated into Rb_{AB}.

(B) Summary of dissociation constants obtained by ITC measurements. The quoted errors are those produced by fitting the data to a two-state model. For the interaction of $E2F_{(243-437)}$ to Rb_{AB} and Rb_{ABC} the affinities are too high to measure reliably and we have therefore quoted the upper limits of the dissociation constants.

Figure 3 – Binding of Fluorescein-E2F, Rhodamine-E2F and Fluorescein-E7 to pRb

Figure 4 – Displacement binding curves: a) $E2F_{409-426}$ peptide; b) detergent

Figure 5 – Screen controls from test screen 6 x 384 plates

Figure 6 – Correlation between inhibition of Rhodamine and Fluorescein-E2F

Figure 7 – Correlation between inhibition of Fluorescein-E2F and Fluorescein-E7

Figure 8 – **a)** Titration curves of rho-N-E2F (n=3); **b)** Time course of the change of fluorescence polarization signal with time taken from a test screen (mean±s.e.m., n=960)

Figure 9 – IC50 curves determined for hits identified using the screening protocol described with reference to Figures 3 to 8: **a)** hit compound IC50 curve; **b)** non-specific inhibitor IC50 curve

Structure determination of pRb/E2F

For crystallisation we used a pRb construct based on that previously described by Lee, J.O., Russo, A.A., and Pavletich, N.P. (1998). Structure of the retinoblastoma tumour-suppressor pocket domain bound to a peptide from HPV E7, Nature 391, 859-65, which has engineered thrombin cleavage sites at the ends of the flexible linker region between the A and B domains. Purification and proteolysis produces a final protein containing residues 372 to 589 of the A domain and 636 to 787 of the B domain (hereafter pRb_{AB} – Figure 1A). Although these two domains are not covalently attached after thrombin treatment, they remain tightly associated. The removal of the A-B linker region facilitates crystallisation of pRb but does not alter its binding affinity for E2F. Crystals of the $pRb/E2F_{(409-426)}$ complex grew in a plate-like

habit with typical dimensions 200 x 200 x 10 μm^3. Repeated attempts at data collection from flash-cooled crystals using synchrotron X-ray sources were thwarted by very high crystal mosaicity and poor data reduction statistics. The problem was overcome by using the micro-focus diffractometer on station ID13 at ESRF current experience and plans at EMBL and ESRF/ID13, Acta Crystallogr D 55, 1765-1770), currently the only such device installed at a synchrotron source. Using a 10x10 μm^2 aperture, data were collected from four separate and widely spaced volumes of a single crystal in order to minimise radiation damage. A total of 100, 1° oscillation images were collected using a MAR CCD detector. These data extended to a Bragg spacing of 2.5 Å with an overall R_{merge} = 9.2%, and completeness of 87%. The structure was solved by molecular replacement and produced initial electron density maps in which the E2F peptide ($E2F_{(409-426)}$) could be readily located.

Protein constructs.

Rb_{AB} was expressed as a GST-fusion protein in *E. coli* using the pGEX-6P vector. The construct was engineered to contain a Prescission protease site at the N-terminus of Rb as well as two thrombin sites (LVPRGS) inserted at either end of the flexible A-B linker. Fusion protein was loaded onto a glutathione Sepharose 4B column before treatment with thrombin and Prescission protease. The resulting eluent was further purified using a Superdex 200 gel filtration column. Rb_{ABC} was expressed in *E. coli* with a C-terminal His-tag using pET-24. Crude lysate was first purified using an S-sepharose column followed by a Ni-NTA step before being run on a Superdex 200 gel filtration column. Recombinant human $E2F1_{(243-437)}$ was expressed in *E. coli* using pGEX-6P with an engineered Prescission protease site at the N-terminus of E2F. Crude lysate was bound onto a glutathione Sepharose 4B column prior to cleavage with the protease. The resulting eluent was further purified by gel filtration on a Superdex 75 column. $E2F_{(409-426)}$ and $E2F_{(380-437)}$ were synthetic peptides. HPV-16 $E7_{(17-98)}$ was prepared as described elsewhere (Clements, A.J., K, Mazzareli, J.M. Ricciardi, R.P. Marmorstein R. (2000). Oligomerization properties of the viral

oncoproteins adenovirus E1A and human papillomavirus E7 and their complexes with the retinoblastoma protein., Biochemistry 39, 16033-16045).

Crystallography.

Plate-like crystals were grown by the hanging drop vapour diffusion method at 4°C. Rb_{AB} was mixed with the E2F-1 peptide at 1:2 molar ratio and concentrated to 15mg/ml. Hanging drops were formed by mixing 1µl of protein solution with an equal volume of reservoir solution containing; 0.14M Na citrate, 26% PEG400, 4% n-propanol and 0.1M Tris at pH 7.8. Crystals were flash frozen in mother-liquor made up to 25% glycerol. Diffraction data were collected using the micro-focus diffractometer at ESRF and processed using the DENZO and SCALEPACK software (Otwinowski, Z.M., W. (1993). In Data Collection and Processing, L.I. Sawyer, N. Bailey, S., ed. (SERC Daresbury Laboratory), pp. 556-562). Molecular replacement calculations were carried out using Amore (CCP4, 1994) with 1GUX.brk as the search model. The final model contains co-ordinates for the protein which cover residues 379-578 of the A domain and 644-787 of the B domain of Rb and the entire $E2F_{(409-426)}$ peptide for the four copies present in the asymmetric unit together with 600 solvent molecules. The refined model has the following residuals; R_{work} =23.7%, R_{free} =28.7%, rmsd bonds = 0.007 Å, rmsd angles =1.3°.

Structure of pRb/E2F complex

The packing of the A and B domains generates a waist-like interface groove into which $E2F_{(409-426)}$ binds in a largely extended manner (Figure 1B). The peptide makes contacts with residues from helices α4, α5, α6, α8 and α9 of domain A, and with α11 from domain B of pRb. Formation of the complex buries 2280 $Å^2$ of surface area, 1500 $Å^2$ of which are hydrophobic. The two end regions of the $E2F_{(409-426)}$ fragment make extensive contacts with pRb, while interactions made by the middle section of the $E2F_{(409-426)}$ fragment (residues 416 to 420) are relatively sparse (Figure 1C). Overall, a high proportion of the hydrogen bond interactions between the two

molecules involves the side chains of conserved pRb residues interacting with the main chain of E2F. Examination of the distribution of conserved residues over the surface of pRb, reveals that the majority are accounted for by the E2F binding site. There is a somewhat smaller cluster of conserved residues associated with the LxCxE binding site. Perhaps the most remarkable aspect of this analysis is that although pRb has been reported to associate with at least 110 cellular proteins perhaps 50 or more in a pocket-dependent manner, the E2F and LxCxE binding sites account for almost all of the conserved residues on its surface. There are two explanations that may partially account for these observations. Firstly, many of the reported binding partners of pRb have yet to be verified. Secondly, the LxCxE binding site is probably responsible for mediating the binding of many different proteins, such as HDAC, to pRb.

Since there are four copies of the pRb/$E2F_{(409-426)}$ complex in the asymmetric unit of our crystal form it is possible both to compare these four crystallographically independent copies of the pRb/$E2F_{(409-426)}$ complex and to compare them with the crystal structure of pRb/E7 without bond E2F (Lee et al., 1998 Supra). The first six residues at the N-terminus, the α3-α4 and α6-α7 loops adopt different conformations between the four copies in our asymmetric unit, while the variations across the rest of the structure between the four molecules is not significant. Comparison of the pRb structure in the presence and absence of bound $E2F_{(409-426)}$ shows that there is essentially no change in the relative orientation of the two lobes of the A/B pocket on $E2F_{(409-426)}$ binding nor any widespread changes in the structures of the individual domains. This comparison does reveal that the end of α4 and the connecting loop to α5 becomes ordered in the pRb/$E2F_{(409-426)}$ complex as two conserved residues (Glu464-pRb & Arg467-pRb located towards the end of α4 in our structure) interact with the $E2F_{(409-426)}$ peptide. Within the $E2F_{(409-426)}$ construct there are eight residues that are conserved across E2F's from all animal species (Figure 1A). Amino-acid substitutions at five of these positions have been shown to lead to loss of binding to pRb but retention of E2F's trans-activation potential. The following description

focuses on the structural role of these five residues. Tyr(411)-E2F appears to play an important role in peptide binding because its phenolic ring occupies a hydrophobic pocket created by Ile(536)-pRb, Ile(532)-pRb, Ile(547)-pRb and Phe(413)-E2F, while its hydroxyl group makes a hydrogen bond to the invariant Glu(554)-pRb. Towards the C-terminal part of the E2F peptide, Leu(424)-E2F and Phe(425)-E2F make several hydrophobic interactions, two of which involve conserved residues. Leu(424)-E2F makes contacts with the aliphatic portion of the side chain of Lys(530)-pRb and also packs against Leu(415)-E2F and Phe(425)-E2F. In addition, Phe(425)-E2F itself packs against Phe(482)-pRb. Unlike the residues of E2F just discussed, the side-chains of Glu(419)-E2F and Asp(423)-E2F do not point into the groove formed between the A and B domains of pRb, but instead point away from it. Glu(419)-E2F hydrogen bonds through a water molecule with the main-chain carbonyl of Thr(645)-pRb; Asp(423)-E2F forms a salt bridge with Arg(467)-pRb located at the end α4.

Finally, as described earlier, the crystal structure shows how E2F makes extensive contacts with largely conserved residues from both the A and B domains of the pocket and that the binding site for E2F is dependent on the structure of the interface between the two domains. This feature of the structure suggests that E2F acts as a sensor of the structural integrity of the pRb pocket. The position and nature of the E2F binding site make the binding of the transcription factor particularly sensitive to mutations in the pocket region of the tumour suppressor protein. The potential significance of these observations will be discussed later with regard to the normal role of pRb in protecting cells against E2F-mediated apoptosis.

Additional determinants of pRb/E2F function

It is clear from a number of studies that, although $E2F_{(409-426)}$ expressed as a Gal4 fusion protein is sufficient to recruit pRb and repress transcription, there are additional interactions made by the physiologically relevant E2F/DP heterodimer with pRb.

Similarly, while the pocket domain is highly conserved, the most frequent site of deleterious mutation, and capable of transcriptional repression, it is not sufficient for the physiological function of pRb. In particular, the C-terminus of pRb is necessary for mediating growth arrest and recruitment of certain cyclin/cdk complexes as well as containing several of the residues whose phosphorylation leads to deactivation of pRb function. Therefore, in order to better understand the requirements for physiological pRb/E2F complex formation, we have made a series of constructs of the two proteins (Figure 1A) and carried out binding measurements by isothermal titration calorimetry (ITC). We have also carried out a series of competition experiments to confirm qualitatively the interpretation of the ITC binding data.

Isothermal Titration Calorimetry.

Binding of the various E2F constructs to Rb_{AB} and Rb_{ABC} was measured by isothermal titration calorimetry using a MicroCal Omega VP-ITC machine (MicroCal Inc., Northampton, USA). The E2F constructs at a concentration between 100-150 μM were titrated into 12-15 μM Rb at a temperature of 22°C. Proteins were dialysed against 50mM Tris pH 7.6, 100mM NaCl and 1mM TCEP. After subtraction of the dilution heats, calorimetric data was analysed using the evaluation software MicroCal Origin v5.0 (MicroCal Software Inc.). For all of the titrations, the stoichiometry of ligand binding to Rb was very close to 1.0. For $E2F_{(243-437)}$ binding to Rb, the binding affinity and the heat change associated with binding were such that we could only establish that binding was tighter than 10 nM. In order to verify that binding of this protein was similar for both Rb_{AB} and Rb_{ABC} we carried out competition experiments which showed approximately equal partition between the two different Rb proteins.

Competition experiments.

The proteins used in these experiments were His_6-Rb_{ABC} (RESIDUES 380-929); MW 66.07kDa, non-tagged Rb_{AB} (residues 372-787); MW 48.67 KDa, are His_6-Rb_{AB} (residues 376-792); MW 49.86 KDa, $E2F_{(243-437)}$; MW 21.45 KDa HPV E7 (residues

17-98); MW 9.38 KDa and $E2F_{(409-426)}$; MW 2.12 KDa. Protein concentrations were carefully determined by u.v. spectroscopy and confirmed by ITC titrations. The small acidic E2F proteins stain much weaker than Rb with Coomassie on SDS-PAGE. For all gel lanes contained a final Rb_{AB} concentration of ca. 7μM. After equilibration with $E2F_{(243-437)}$ and $E2F_{(409-426)}$ the samples were loaded onto a 1.0ml Ni column and washed with 7 x 0.5 ml of loading buffer (50mM Tris pH 7.5, 200mM NaCl & 10mM Imidazole). The samples were then eluted with 7 x 0.5ml elution buffer (50mM Tris, pH 7.5, 200mM NaCl, 200mM Imidazole). After volume correction samples were boiled in SDS loading buffer and run on a 4-12% SDS PAGE. For the two pRb proteins and $E2F_{(243-437)}$ were mixed at 40μM in a final volume of 0.5ml. After equilibration for 2hrs the mixture was loaded onto 1ml Ni beads in a small column, washed with 7 x 0.5ml of loading buffer (50mM Tris, pH 7.5, 200mM NaCl, 10mM Imidazole), eluted using 7 x 0.5ml elution buffer (50mM Tris, pH 7.5, 200mM NaCl, 200mM Imidazole). Samples, after correcting for volume were boiled in SDS sample buffer and run on a 4-12% SDS gel.

A typical ITC experiment is shown in Figure 2A and a summary of the affinity constants obtained for both pRb_{AB} and pRb_{ABC} interacting with three constructs of E2F are given in Figure 2B. The two shorter E2F constructs bind to either pRb_{AB} or pRb_{ABC} with similar affinities. However, $E2F_{(243-437)}$ binds at least 16-fold stronger than either of the two shorter E2F fragments to both pRb_{AB} and Rb_{ABC}. Our ITC data therefore show that there are additional interactions of the A/B pocket of pRb with a region of E2F-1 outside of the transactivation domain. This result has been confirmed qualitatively by competition experiments which show that a 15-to 30-fold molar excess of the shorter E2F peptide is required to 50% compete with $E2F_{(243-437)}$ for binding to pRb. Our results are consistent with an earlier report that noted an interaction of pRb with the marked box region of E2F (residues 245-317). Taken together, these data demonstrate that the majority of the free energy of interaction between pRb and E2F is contributed by the 18-residue segment $E2F_{(409-426)}$ used in our

structure analysis. There is an additional stabilising interaction between the marked box region of E2F and pRb, that contributes approximately 2kcal mol^{-1} to the overall free energy of complex formation, but is not sufficient on its own for complex formation.

As the binding constant for the interaction of $E2F_{(243-437)}$ with pRb_{AB} (or pRb_{ABC}) was too tight to determine reliably by ITC we performed a competition experiment to determine if this E2F construct bound preferentially to one or the other pRb construct. The results show approximately equal partitioning of $E2F_{(243-437)}$ between the two pRb species and demonstrates therefore, that the C-terminus of pRb does not participate in the binding to E2F-1 in isolation. This means that in addition to the interaction of $E2F_{(409-426)}$ with the pocket region of pRb there is an additional interaction, almost certainly involving the marked box region of E2F, that also binds to the pRb pocket. This data is consistent with the hypothesis that the approximately 10-fold stronger interaction of E2F/DP with pRb_{ABC} rather than pRb_{AB} reported previously arises through interactions of the DP component of the E2F/DP heterodimer with the C-terminus of pRb. This idea is strongly supported by the data from another study which shows that DP-1 interacts with pRb in a manner that does not require the structural integrity of the A/B pocket. Taken together, these data indicate that at least one of the functions of the C-terminus of pRb is to bring additional stabilisation to the interaction of the tumour suppressor with the heterodimeric E2F/DP transcription factors.

Use of structure atomic co-ordinates of Annex I

The atomic co-ordinates of Annex 1 are cartesian co-ordinates derived from the results obtained on diffraction of a monochromatic beam of X-rays by the atoms of the pRb/ $E2F_{(409-26)}$ complex in crystal form. The diffraction data was used to calculate electron density maps of the crystal. The electron density maps were then used to position the individual atoms of the pRb/ $E2F_{(409-26)}$ complex.

The determination of the three-dimensional structure of the pRb/E2F$_{(409-426)}$ complex provides basis for the design of new and specific agents that modulates formation of the complex and/or modulates the interaction between pRb and E2F$_{(409-426)}$. For example, computer modelling programs may be used to design different molecules expected to modulate formation of the pRb/E2F$_{(409-426)}$ complex and/or the interactions between pRb and E2F$_{(409-426)}$.

A candidate agent, may be any available compound. A commercial library of compound structures such as the Cambridge Structural Database would enable computer based *in silico* screening of the databases to enable compounds that may interact with, and/or modulate formation of, the complex to be identified.

Such libraries may be used to allow computer-based high throughput screening of many compounds in order to identify and select those agents with potential to modulate formation of the pRb/E2F$_{(409-426)}$ complex and/or the interaction between pRb and E2F$_{(409-426)}$.

In this regard, a potential modulating agent can be subjected to computer modelling with a docking program such as GRAM, DOCK or AUTODOCK (see Walters et al., Drug discovery Today, Vol.3, No. 4, (1998), 160-178, and Dunbrack et al., Folding and Design, 2 (1997) 27-42) to identify and select potential agents. This can include computer fitting of potential modulating agents to the pRb/E2F$_{(409-426)}$ complex to ascertain how the agent, in terms of shape and structure, will bind to the complex.

Computer programs can be employed to estimate the interactions between the pRb, E2F$_{(409-426)}$ and agent or pRb/E2F$_{(409-426)}$ complex and agent. These interactions may be attraction, repulsion, and steric hindrance of the two binding partners (e.g. the pRb/E2F$_{(409-426)}$ complex and a selected agent). A potential agent will be expected to be more potent if there is a tighter fit and fewer steric hindrances, and therefore greater attractive forces.It is advantageous for the agent to be specific to reduce interaction

with other proteins. This could reduce the occurrence of side-effects due to additional interactions with other proteins.

Potential agents that have been designed or selected possible agents can then be screened for activity as set out in the second to tenth aspects above. The agents can be obtained from commercial sources or synthesised. The agent is then contacted with pRb/E2F$_{(409-426)}$ complex to determine the ability of the potential agent to modulate the formation of the complex. Alternatively the agent may be contacted with pRb and E2F$_{(409-426)}$ under conditions in which pRb and E2F$_{(409-426)}$ can form a complex (in the absence of agent), to determine the ability of the agent to modulate complex formation.

A complex of pRb/E2F$_{(409-426)}$ and said potential agent can then be formed such that the complex can be analysed by X-ray crystallography to determine the ability of the agent to modulate complex formation and/or the interaction between pRb and E2F$_{(409-426)}$.

The complex of pRb/E2F$_{(409-426)}$ and agent could be compared to that for pRb/E2F$_{(409-426)}$ alone with the three dimensional atomic co-ordinates in Annex 1.

Detailed structural information can then be obtained about the binding of the potential agent to the complex,. This will enable the structure or functionality of the potential agent to be altered to thereby to improve binding. The above steps may be repeated as may be required.

The agent-pRb/E2F$_{(409-426)}$ complex could be analysed by co-crystallising pRb/E2F$_{(409-426)}$ with the selected agent or soaking the agent into crystals of the pRb/E2F$_{(409-426)}$ complex; and then determining the three dimensional co-ordinates of the agent-complex by X-ray diffraction using molecular replacement analysis.

Therefore, the pRb/E2F$_{(409-426)}$ -agent complexes can be crystallised and analysed using X-ray diffraction data obtained and processed, for example using the DENZO and SCALEPACK software (Otwinowksi, Z. M., W. (1993). Difference Fourier electron density maps can be calculated based on X-ray diffraction patterns of soaked or co-crystallised pRb/E2F$_{(409-426)}$ complex and the solved structure of uncomplexed agent. These maps can then be used to determine the structure of the agent bound to the pRb/E2F$_{(409-426)}$ and/or changes in the conformation of pRb/E2F$_{(409-426)}$ complex relative to the pRb/E2F$_{(409-426)}$ complex in the absence of agent.

The agent may be improved, for example by adding or removing functional groups, substituting groups or altering its shape in light of data obtained from agent bound to pRb/E2F$_{(409-426)}$ complex and/or agent bound to pRb. Such an improved agent may then be subjected to the methods of the invention.

Electron density maps can be calculated using programs such Amore from the CCP4 computing package (Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, Acta Crystallographical, D50, (1994), 760-763).

The provision of computer readable media enables the atomic co-ordinates to be accessed to model the pRb/E2F$_{(409-426)}$ complex by, for example, RAMSOL (a publicly available computer software package which allows access and analysis of atomic co-ordinate data for structure determination and/or rational drug design).

In addition, structure factor data, derivable from the atomic co-ordinate data (see e.g. Blundell et al., in Protein Crystallography, Academic Press, New York, London and San Francisco, (1976)), can be used to enable difference Fourier electron density maps to be deduced.

Screening assays

After an agent has been selected, its inhibitory effect on pRb/$E2F_{(409-426)}$ complex formation or ability to interact with the pRb/$E2F_{(409-426)}$ complex can be assessed with one or more of the methods of the invention.

For example, the crystal structure of the interaction of $E2F_{(409-426)}$ with pRb can be used to aid the design of a fluorescently tagged peptide for the use in a binding assay suitable for high throughput screening of low molecular weight compounds or peptide libraries. The fluorescent tag may be a fluorescein, rhodamine or some other commercially available tag chemically attached via a suitable amine or thiol group.

Binding could be measured by detecting fluorescence polarization in an homogeneous assay format (i.e. one in which all reagents are mixed in a single well, and reaction occurs in solution without wash steps). Fluorescence polarization technology is commonly applied in high throughput screening laboratories (ref: Sokham et al. (1999) Analytical Biochemistry, 275, 156-161. "Analysis of protein-peptide interaction by a miniaturised fluorescence polarization assay using cyclin-dependent kinase2/cyclin E as a model system.")

Fluorescence polarization can be used to determine binding of a fluorescently- tagged small molecule (ligand or peptide) with a large molecule (receptor or protein) by detecting changes in the rotational velocity of the small molecule in the free and bound state. The rotational velocity is inversely proportional to the size of the molecule. Using a fluorescently tagged peptide and suitable optics the changes in rotational velocity upon binding to pRb can be measured as a differences in light emitted in parallel and perpendicular to a polarized excitation source. Fluorescence polarisation gives a measure of the proportion of fluorescently tagged peptide found in the bound state in a homogenous format.

In an assay method of the present invention, fluoro-peptide ($E2F_{(409-426)}$–fluoropeptide) bound to pRb will have a low rotational velocity and will appear

stationary during the excitation period. Emitted light will be transmitted in parallel to the polarized incident light and the light detected will have a high polarization value. In contrast in the presence of an inhibitor of the interaction between pRb and $E2F_{(409-426)}$-fluoropeptide, the free $E2F_{(409-426)}$- fluoro-peptide will have a high rotational velocity and light will be transmitted in all directions. Emitted light will be detected both parallel and perpendicular to the polarized excitation source, and will have a low polarization value.

An example of the use of fluorescence polarisation is now described.

Data from a Fluorescence Polarisation (FP) screen configured for the interaction of pRb with E2F is presented. Fluorescein-tagged E2F peptide was used to screen 10,000 small drug like molecules. Hit confirmation strategies based on fluorescence interference and specificity were developed and compared.

Based on the crystal structure defined by the atomic co-ordinates in Annex 1, an FP screen was configured for the interaction of recombinant pRb A/B domains with E2F(409-426) peptide (see Fig 1B). In addition, a second peptide binding site (E7, see Fig 1B), distant from the E2F binding pocket, was utilised as an internal control for non-specific inhibitors. Fluorophores in the form of fluorescein and rhodamine labelled peptides were synthesised and were used in a primary screen and hit confirmation.

Knowledge of the interaction of E2F and E7 peptides with pRb influenced the design of the fluoro-peptides used in the assay. The following peptides were synthesised, labelled and tested.

1. N-terminal amide linkage 5carboxyfluorescein-E2F409-426, 18'mer. (fl-N-E2F18)

LDYHFGLEEGEGIRDLFD

2. Rhodamine label at C-terminal cysteine E2F409-427, 19'mer. (Rh-C-E2F19)

LDYHFGLEEGEGIRDLFDC

3. Rhodamine label at DDC substitution E2F409-426, 18'mer. (Rh-N2-E2F18)

LCYHFGLEEGEGIRDLFD

4. N-terminal amide linkage 5carboxyfluorescein-E7, nonomer (Fl-E7)

DLYCYEQLN

Peptides 1, 3 and 4 were used in the screen and subsequent hit confirmation assays.

Synthetic peptides were synthesised and fluoro-tagged using either N-terminal labelling with 5 carboxyfluorescein succinimidyl ester or cysteine labelling with single isomer tetramethylrhodamine-5- maleimide. Typical titration binding curves of pRb with the fluoro-labelled peptides are shown (mean±sem, n=3) in Figure 3. Fluorescein fluorescence measured at λexcite = 485 and λemit = 520 nm
Rhodamine fluorescence measured at λexcite = 545 and λemit = 580 nm

Measurements were made using BMG Fluorostar plate reader fitted with polarization optic. Fluorescein-E2F showed the greatest degree of polarization, and consequently the best signal to noise. It was chosen as the label of choice for a primary screen. Data were fitted to a one site binding model using Graphpad prism. Kd values of

450± 70 and 380±50 nM were calculated for fluorescein and Rhodamine labelled E2F, which were similar to Kd determined for unlabelled peptide using isothermal calorimetry. Fluorescein-E7 showed tightest binding with Kd= 130±20 nM.

The assay principle was validated using unlabelled E2F peptide to displace Fl-E2F without disrupting Fl-E7 binding to pRb. Fluoro-tagged peptide (400 nM) was pre-incubated with pRb (1 μM) and unlabelled peptide added at the concentrations shown. Displacement binding curves were plotted (figure 4a), and were fitted to a one site competition binding model using Graphpad prism curve fitting software. These curves were compared to the effects of a detergent-like compound (figure 4b), which causes gross structural changes and disrupts binding of both peptides.

The results show that labelled E2F (Fl-E2F) does not displace E7, thereby validating the assay principle.

The assay was optimised in 384-well black plates (Matrix) and automated using a Beckman Fx liquid handling robot. 1 μM pRb in 50 mM Tris HCL, pH7.0, 100 mM NaCl, 10 mM DTT, 0.05% NP-40 was mixed with 40 μM compound (4% DMSO) and 0.4 μM fluorescein-E2F (final concentrations). Controls from a test screen of 10,000 compounds are shown in Figure 5.

Polarized and depolarized signal from fluorescein-E2F with and without pRb present are shown in Figure 5 (solid and open circles respectively). Specific disruption of binding by E2F protein and peptide are also shown. Addition of E2F protein completely displaces Fl-E2F (open triangle) and the signal is reduced to that of free fluoro-peptide alone. Addition of unlabelled-E2F at a concentration which gave 50% inhibition is clearly separated from the control populations. Hits were identified as compounds which reduced the polarization signal to less than mean-3sd of the fluorescein-E2F: pRb control.

Summary of Screen Data

Assay Principle		Fluorescence Polarization
Assay Automation		Biomek Fx
Assay Detection		BMG Polar Star Reader
Assay Parameters	Signal: noise	6.9
	Signal: background	4.8
	Z`	0.67
Test Screen 10,000	Z	0.45
	Hit rate	0.93%

Z factors are statistical factors well known by the skilled person in the art. The Z' factor is defined by

$$Z` = 1 - \left(\frac{(3X \text{ s.d.of positive control} + 3X \text{ s.d of negative control})}{(\text{mean of positive control} - \text{mean of negative control})} \right)$$

In the present assay:-
positive control = fully polarized signal; pRb plus fluoro-tagged E2F peptide
negative control = depolarized signal from fluoro-tagged E2F peptide alone.

Z is calculated in much the same way except:
Positive control = polarized signal of pRb and fluoro-tagged E2F in presence of compounds.

HIT CONFIRMATION:

Identification of Fluorescence Interfering Compounds.

A large proportion (37.5%) of the hits selected from the primary screen were coloured compounds which significantly altered the fluorescence intensity signal, and were potentially interfering with the assay. All hits were included in hit confirmation assays.

Hits were re-plated from master stocks and re-tested against fluorescein-E2F and rhodamine-E2F. A correlation (r^2=0.69) between inhibition of fluorescein E2F and Rhodamine-E2F was observed (figure 6) with a hit confirmation rate of 78%. Notably, 60% of compounds which were potentially interfering with the fluorescein signal were inhibitors with Rhodamine-E2F assay, without affecting rhodamine fluorescence intensity signal. Suggesting that deselection of compounds on the basis of fluorescence interference can lead to loss of real inhibitors.

Finally the hits were tested against a second peptide binding site. Fluorescein-E7 peptide at 400 nM. The results were compared to inhibition of E2F and a scatter plot is shown in Figure 7. A weak correlation was observed (r^2=0.51), with 72% of the inhibitors of E2F also inhibiting fluorescein E7. These compounds were excluded as non-specific inhibitors and were not taken forward in subsequent biochemical assays.

Comparison of Hit Confirmation Strategies on 80 best hits selected from a Primary screen of 10,000 compounds.

Hit Confirmation rates

Confirmation Test	% Primary Hits
1. Inhibition in retest Fluorescein-E2F	77.5
2. Fluorescence Interference	37.5
3. Inhibition in retest Rhodamine-E2F	62.5
4. Inhibition of Fluorescein-E7	58.5

The impact of selection strategy on number of compounds selected for further biochemical study (eg IC50, isothermal calorimetry, co-crystallisation)

Strategy 1	Strategy 2	Strategy 3
Tests 1+2 Remove fluorescence interfering compounds 36	Tests 1+3 Select inhibitors active for both fluorescein- and rhodamine-E2F 50	Tests 1+3+4 E2F inhibitors but not E7 inhibitors 14
False Negatives	False Positives	Specific Compounds only

To demonstrate the stability and rapidity of binding equilibria of fluoro-peptide with pRb. The titration curves shown in Figures 8a and 8b are typical of several experiments and are of rho-N-E2F (n=3). The time course shown of the change of fluorescence polarization signal with time is taken from a test screen (mean ± s.e.m., n= 960).

pRb titration curves were performed in 96-well black plates, in a total reaction volume of 100uL. Doubling dilutions from 10 μM stock of pRb were made in binding buffer (50 mM Tris HCL, pH7.0, 100 mM NaCl, 10 mM DTT, 0.05% NP-40) and 80 μL added in triplicate to wells. 20 μL of 2 μM fluoro-peptide was added and pipetted up and down to mix. The plate was read after 1 hr incubation at room temperature.

Compound interference was not a useful factor upon which to deselect compounds in an FP assay, and can lead to false negatives. The use of a second fluoro-label in hit confirmation avoids the loss of false negatives, but still includes false positives.

Screening of the hits against the second peptide site, E7, identified non-specific inhibitors, which caused gross structural changes to the protein. These were excluded from further biochemical testing. Identification of these non-specific inhibitors dramatically reduced the down stream work load.

The developed screening strategy rapidly identifies false negatives and positives (interfering and protein unfolding reagents) from the primary screen. This reduces the number of compounds to test in biochemical assays, thus saving both time and reagents which will accelerate the hit to lead discovery process.

ANS (aniline naphthalene sulphonic acid) reagent may be used to detect hydrophobic surfaces on pRb which become exposed as it unfolds. The fluorescence of ANS is highly sensitive to its environment. In solution there is virtually no fluorescence, whereas when bound to protein, such as pRb, it fluoresces highly. Changes in protein structure can alter the fluorescent signal of bound ANS due to changes in its environment to water. Therefore changes in pRb structure can be detected on addition of ANS and the agent that modulates pRb/E2F$_{(409-426)}$ complex. If the fluorescent signal alters on addition of the agent, the agent may be affecting the pRb structure. The use of ANS to monitor protein unfolding is known in the art (Semisotnov et al (1991) Biopolymers, 31(1), 119-128)

Biochemical assays could include IC50, isothermal calorimetry, and/or co-crystallisation.

In an example of an IC50 assay, reactions were performed in 96-well black plates in a total reaction volume of 100 µL. Compounds were dissolved in DMSO at a maximum concentration of 10 mM and doubling dilutions made in DMSO. 4 µL of diluted compound was mixed with 80 µL pRb (400 nM in binding buffer). The plate was incubated at room temperature for 15 min and then Rhodamine-E2F and fluorescein-

E7 were added to give final concentrations of 400 nM each. Reactions were performed in triplicate. Plates were read after 1 hr. The results are shown in Figures 9a and 9b.

Accordingly, an assay method could include the following steps:

a) allow complex formation of pRb and $E2F_{(409-426)}$-fluoropeptide, and measure maximum fluorescence polarization; and
b) add a selected agent and detect whether there is a decrease in fluorescence polarization.

Alternatively, an assay method could include the steps:

a) allow complex formation of pRb and $E2F_{(409-426)}$-fluoropeptide in the presence and absence of a selected agent and measure the fluorescence polarization; and
b) compare the fluorescence polarization values.

Compounds which stabilise the pRb/$E2F_{(409-426)}$ complex could be assessed in a modification of the above method, involving competition binding of pRb by unlabelled $E2F_{(409-426)}$ and $E2F_{(409-426)}$-fluoropeptide.

In this regard an assay method could include the following steps:

a) allow complex formation of pRb/$E2F_{(409-426)}$-fluoropeptide, and measure max fluorescence polarization;
b) add a selected agent and measure fluorescence polarization - if no change in fluorescence polarization there is no disruption of complex;
c) add unlabeled $E2F_{(409-426)}$ and measure fluorescence polarization - expect displacement of $E2F_{(409-426)}$-fluoropeptide and a decrease in fluorescence polarization, but not if complex is stabilised by presence of the agent.

Alternatively, the pRb, $E2F_{(409-426)}$-fluoropeptide and agent could be added together before detecting fluorescence polarization. If fluorescence polarization is reduced to

less than a predetermined value, the agent is determined to destabilize the complex, and vice versa.

The interactions could be confirmed by co-crystalisation of pRb/$E2F_{(409-426)}$ with the agent, and determination of the three dimensional atomic coordinates by X-ray diffraction and molecular replacement.

The $E2F_{(409-426)}$/pRb interaction can also be applied to heterogeneous assay formats (i.e. ones in which reagents are partitioned between a solid support and in solution, and wash steps are involved). This would involve the immobilisation of pRb on microtitre plates, for example by antibody capture or metal ion chelation using His-tagged pRb and Nickel coated plates. $E2F_{(409-426)}$ peptide may be tagged with fluorescence as above and the fluorescence detected directly to determine binding. Alternatively, the peptide could be labelled with biotin and detected with streptavidin-horse radish peroxidase in an ELISA-like format.

Compounds which interact with the complex without altering association or disassociation of the complex could be identified by crystallographic means, unless the agent itself was tagged (radioactivity/fluorescence) and binding to the complex measured directly, eg fluorescence polarization as above or scintallation counting of an immuno-precipitate.

Alternatively, the agent can be added to pRb and $E2F_{(409-26)}$ under conditions in which pRb and $E2F_{(409-26)}$ can form a complex. This could result in the agent and complex co-crystallising. The binding affinities of pRb to $E2F_{(409-26)}$ in the pRb/ $E2F_{(409-26)}$ complex in the presence and absence of the agent can then be compared to determine whether the agent inhibits complex formation. The three dimensional structure of the pRb/ $E2F_{(409-26)}$ – agent complex can also be solved (X-ray diffraction using molecular replacement analysis) to enable the associations in the new complex to be compared with those in the pRb/ $E2F_{(409-26)}$ complex (see Annex 1). As a further alternative the

pRb/ $E2F_{(409-26)}$ complex can be formed before soaking the complex in the presence of a selected agent. The binding affinities of pRb to $E2F_{(409-26)}$ can then be determined in the presence and absence of the agent. As before, the three dimensional structure of any pRb/ $E2F_{(409-26)}$ – agent complex could be solved.

The binding affinities can be measured using isothermal titration calorimetry. Alternatively, surface plasmon resonance (SPR) could be used such as that provided by Biacore AB.

Preferred features of each aspect of the invention are as for each of the other aspects *mutatis mutandis*. The prior art documents mentioned herein are incorporated to the fullest extent permitted by law.

Annex 1

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REMARK the coordinates is one molecule from four molecules in an asymmetric
REMARK unit cell whithin the crystal:
REMARK a=101.996  b=158.548  c=110.617  alpha=90.00  beta=93.70  gama=90.00 C 2
ATOM      1  N   MET A 379      13.261 -15.752  30.447  1.00 45.11           N
ATOM      2  CA  MET A 379      11.983 -16.486  30.626  1.00 44.12           C
ATOM      3  CB  MET A 379      11.935 -17.082  32.026  1.00 44.57           C
ATOM      4  CG  MET A 379      12.067 -16.066  33.137  1.00 45.87           C
ATOM      5  SD  MET A 379      12.458 -16.814  34.740  1.00 52.60           S
ATOM      6  CE  MET A 379      10.805 -17.831  35.114  1.00 52.37           C
ATOM      7  C   MET A 379      10.802 -15.543  30.446  1.00 43.32           C
ATOM      8  O   MET A 379       9.681 -15.889  30.824  1.00 43.69           O
ATOM      9  N   ASN A 380      11.069 -14.348  29.909  1.00 41.45           N
ATOM     10  CA  ASN A 380      10.043 -13.347  29.646  1.00 39.85           C
ATOM     11  CB  ASN A 380      10.641 -11.934  29.700  1.00 39.85           C
ATOM     12  CG  ASN A 380      10.867 -11.446  31.134  1.00 40.80           C
ATOM     13  OD1 ASN A 380       9.924 -11.442  31.937  1.00 40.97           O
ATOM     14  ND2 ASN A 380      12.115 -11.037  31.461  1.00 36.52           N
ATOM     15  C   ASN A 380       9.449 -13.550  28.273  1.00 38.62           C
ATOM     16  O   ASN A 380      10.144 -14.006  27.355  1.00 38.16           O
ATOM     17  N   THR A 381       8.174 -13.193  28.126  1.00 36.87           N
ATOM     18  CA  THR A 381       7.530 -13.259  26.812  1.00 35.53           C
ATOM     19  CB  THR A 381       6.303 -14.214  26.805  1.00 35.83           C
ATOM     20  OG1 THR A 381       5.350 -13.786  27.792  1.00 37.01           O
ATOM     21  CG2 THR A 381       6.717 -15.621  27.249  1.00 35.34           C
ATOM     22  C   THR A 381       7.123 -11.901  26.289  1.00 33.36           C
ATOM     23  O   THR A 381       6.745 -11.028  27.043  1.00 32.65           O
ATOM     24  N   ILE A 382       7.170 -11.770  24.971  1.00 31.97           N
ATOM     25  CA  ILE A 382       6.820 -10.549  24.266  1.00 30.21           C
ATOM     26  CB  ILE A 382       6.724 -10.881  22.782  1.00 30.35           C
ATOM     27  CG1 ILE A 382       6.672  -9.609  21.938  1.00 29.02           C
ATOM     28  CD1 ILE A 382       7.902  -8.721  22.081  1.00 33.06           C
ATOM     29  CG2 ILE A 382       5.534 -11.833  22.531  1.00 28.36           C
ATOM     30  C   ILE A 382       5.498 -10.020  24.767  1.00 29.89           C
ATOM     31  O   ILE A 382       5.258  -8.833  24.884  1.00 30.56           O
ATOM     32  N   GLN A 383       4.638 -10.942  25.092  1.00 29.58           N
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ATOM     33  CA  GLN A 383       3.305 -10.639  25.574  1.00 29.76           C
ATOM     34  CB  GLN A 383       2.535 -11.945  25.820  1.00 29.93           C
ATOM     35  CG  GLN A 383       1.103 -11.705  26.237  1.00 34.71           C
ATOM     36  CD  GLN A 383       0.261 -12.955  26.137  1.00 39.96           C
ATOM     37  OE1 GLN A 383      -0.945 -12.917  26.383  1.00 39.55           O
ATOM     38  NE2 GLN A 383       0.895 -14.071  25.754  1.00 43.51           N
ATOM     39  C   GLN A 383       3.155  -9.723  26.795  1.00 27.99           C
ATOM     40  O   GLN A 383       2.247  -8.901  26.822  1.00 27.26           O
ATOM     41  N   GLN A 384       4.019  -9.868  27.792  1.00 26.56           N
ATOM     42  CA  GLN A 384       3.915  -9.050  28.974  1.00 24.94           C
ATOM     43  CB  GLN A 384       4.648  -9.689  30.147  1.00 26.49           C
ATOM     44  CG  GLN A 384       6.156  -9.957  30.006  1.00 29.94           C
ATOM     45  CD  GLN A 384       6.694 -10.838  31.188  1.00 35.67           C
ATOM     46  OE1 GLN A 384       6.215 -11.970  31.425  1.00 33.73           O
ATOM     47  NE2 GLN A 384       7.677 -10.306  31.921  1.00 37.23           N
ATOM     48  C   GLN A 384       4.371  -7.617  28.771  1.00 23.54           C
ATOM     49  O   GLN A 384       3.720  -6.670  29.241  1.00 23.14           O
ATOM     50  N   LEU A 385       5.466  -7.419  28.053  1.00 21.30           N
ATOM     51  CA  LEU A 385       5.894  -6.053  27.840  1.00 19.42           C
ATOM     52  CB  LEU A 385       7.244  -5.976  27.128  1.00 20.05           C
ATOM     53  CG  LEU A 385       7.786  -4.583  26.770  1.00 20.09           C
ATOM     54  CD1 LEU A 385       7.807  -3.617  27.986  1.00 16.89           C
ATOM     55  CD2 LEU A 385       9.205  -4.708  26.201  1.00 22.07           C
ATOM     56  C   LEU A 385       4.848  -5.381  26.989  1.00 18.64           C
ATOM     57  O   LEU A 385       4.598  -4.175  27.168  1.00 17.76           O
ATOM     58  N   MET A 386       4.253  -6.140  26.050  1.00 16.78           N
ATOM     59  CA  MET A 386       3.192  -5.561  25.195  1.00 16.27           C
ATOM     60  CB  MET A 386       2.769  -6.488  24.033  1.00 16.13           C
ATOM     61  CG  MET A 386       3.278  -6.115  22.679  1.00 14.44           C
ATOM     62  SD  MET A 386       2.985  -7.361  21.343  1.00 20.61           S
ATOM     63  CE  MET A 386       1.260  -6.895  20.591  1.00 17.31           C
ATOM     64  C   MET A 386       1.953  -5.117  26.014  1.00 15.44           C
ATOM     65  O   MET A 386       1.304  -4.152  25.688  1.00 14.45           O
ATOM     66  N   MET A 387       1.641  -5.823  27.085  1.00 14.99           N
ATOM     67  CA  MET A 387       0.500  -5.451  27.907  1.00 15.36           C
ATOM     68  CB  MET A 387       0.080  -6.634  28.771  1.00 16.60           C
ATOM     69  CG  MET A 387      -0.663  -7.709  28.039  1.00 21.28           C
ATOM     70  SD  MET A 387      -1.472  -8.842  29.235  1.00 33.36           S
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ATOM     71  CE  MET A 387      -0.081  -9.970  29.834  1.00 29.39           C
ATOM     72  C   MET A 387       0.815  -4.229  28.810  1.00 13.51           C
ATOM     73  O   MET A 387      -0.019  -3.369  29.075  1.00 12.21           O
ATOM     74  N   ILE A 388       2.043  -4.183  29.273  1.00 11.97           N
ATOM     75  CA  ILE A 388       2.515  -3.099  30.071  1.00 10.08           C
ATOM     76  CB  ILE A 388       3.933  -3.432  30.575  1.00 11.21           C
ATOM     77  CG1 ILE A 388       3.834  -4.616  31.556  1.00 10.61           C
ATOM     78  CD1 ILE A 388       5.163  -5.022  32.182  1.00 14.30           C
ATOM     79  CG2 ILE A 388       4.646  -2.204  31.211  1.00  9.99           C
ATOM     80  C   ILE A 388       2.484  -1.844  29.271  1.00  8.68           C
ATOM     81  O   ILE A 388       1.938  -0.883  29.723  1.00 10.11           O
ATOM     82  N   LEU A 389       3.028  -1.833  28.060  1.00  7.85           N
ATOM     83  CA  LEU A 389       3.047  -0.600  27.248  1.00  6.29           C
ATOM     84  CB  LEU A 389       4.037  -0.694  26.100  1.00  5.90           C
ATOM     85  CG  LEU A 389       5.546  -0.953  26.392  1.00  5.99           C
ATOM     86  CD1 LEU A 389       6.365  -0.770  25.087  1.00  2.00           C
ATOM     87  CD2 LEU A 389       6.148  -0.133  27.549  1.00  4.06           C
ATOM     88  C   LEU A 389       1.681  -0.189  26.740  1.00  6.09           C
ATOM     89  O   LEU A 389       1.326   0.998  26.635  1.00  5.28           O
ATOM     90  N   ASN A 390       0.872  -1.196  26.489  1.00  6.69           N
ATOM     91  CA  ASN A 390      -0.485  -0.947  26.080  1.00  7.16           C
ATOM     92  CB  ASN A 390      -1.197  -2.234  25.755  1.00  6.39           C
ATOM     93  CG  ASN A 390      -1.054  -2.597  24.310  1.00  8.37           C
ATOM     94  OD1 ASN A 390      -0.467  -1.844  23.505  1.00  7.04           O
ATOM     95  ND2 ASN A 390      -1.582  -3.753  23.948  1.00 11.15           N
ATOM     96  C   ASN A 390      -1.269  -0.146  27.084  1.00  7.15           C
ATOM     97  O   ASN A 390      -2.038   0.694  26.653  1.00  9.07           O
ATOM     98  N   SER A 391      -1.074  -0.344  28.385  1.00  6.14           N
ATOM     99  CA  SER A 391      -1.849   0.461  29.338  1.00  7.59           C
ATOM    100  CB  SER A 391      -2.517  -0.391  30.413  1.00  7.30           C
ATOM    101  OG  SER A 391      -1.555  -1.006  31.241  1.00  6.73           O
ATOM    102  C   SER A 391      -1.091   1.626  30.005  1.00  7.70           C
ATOM    103  O   SER A 391      -1.696   2.512  30.608  1.00  6.83           O
ATOM    104  N   ALA A 392       0.233   1.610  29.872  1.00  8.42           N
ATOM    105  CA  ALA A 392       1.082   2.673  30.415  1.00  7.80           C
ATOM    106  CB  ALA A 392       2.494   2.367  30.091  1.00  6.49           C
ATOM    107  C   ALA A 392       0.695   4.043  29.860  1.00  8.43           C
ATOM    108  O   ALA A 392       0.169   4.150  28.755  1.00  8.78           O
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ATOM    109  N   SER A 393       0.958   5.087  30.638  1.00 10.46           N
ATOM    110  CA  SER A 393       0.655   6.482  30.310  1.00 11.12           C
ATOM    111  CB  SER A 393       0.692   7.253  31.571  1.00 11.04           C
ATOM    112  OG  SER A 393       0.415   8.586  31.290  1.00 15.76           O
ATOM    113  C   SER A 393       1.651   7.157  29.385  1.00 12.00           C
ATOM    114  O   SER A 393       2.838   6.842  29.408  1.00 13.27           O
ATOM    115  N   ASP A 394       1.167   8.108  28.595  1.00 11.46           N
ATOM    116  CA  ASP A 394       1.987   8.875  27.679  1.00 11.53           C
ATOM    117  CB  ASP A 394       1.133   9.445  26.524  1.00 10.85           C
ATOM    118  CG  ASP A 394       0.624   8.353  25.569  1.00 15.82           C
ATOM    119  OD1 ASP A 394       1.378   7.926  24.658  1.00 17.94           O
ATOM    120  OD2 ASP A 394      -0.509   7.835  25.673  1.00 18.22           O
ATOM    121  C   ASP A 394       2.686  10.030  28.391  1.00 11.56           C
ATOM    122  O   ASP A 394       3.497  10.760  27.796  1.00 12.74           O
ATOM    123  N   GLN A 395       2.383  10.206  29.656  1.00 10.33           N
ATOM    124  CA  GLN A 395       2.922  11.325  30.369  1.00 10.45           C
ATOM    125  CB  GLN A 395       1.740  12.142  30.905  1.00 11.83           C
ATOM    126  CG  GLN A 395       0.976  12.872  29.792  1.00 14.78           C
ATOM    127  CD  GLN A 395       1.927  13.681  28.846  1.00 17.31           C
ATOM    128  OE1 GLN A 395       1.612  13.884  27.668  1.00 13.52           O
ATOM    129  NE2 GLN A 395       3.073  14.156  29.388  1.00 15.32           N
ATOM    130  C   GLN A 395       3.822  10.878  31.519  1.00  8.54           C
ATOM    131  O   GLN A 395       3.698   9.784  32.001  1.00  7.56           O
ATOM    132  N   PRO A 396       4.735  11.724  31.946  1.00  7.59           N
ATOM    133  CA  PRO A 396       5.567  11.391  33.102  1.00  8.16           C
ATOM    134  CB  PRO A 396       6.401  12.675  33.324  1.00  6.76           C
ATOM    135  CG  PRO A 396       6.360  13.350  32.081  1.00  6.09           C
ATOM    136  CD  PRO A 396       5.063  13.040  31.373  1.00  6.71           C
ATOM    137  C   PRO A 396       4.665  11.077  34.336  1.00  8.69           C
ATOM    138  O   PRO A 396       3.600  11.699  34.508  1.00  9.77           O
ATOM    139  N   SER A 397       5.084  10.162  35.184  1.00  8.42           N
ATOM    140  CA  SER A 397       4.221   9.811  36.311  1.00  9.96           C
ATOM    141  CB  SER A 397       4.561   8.437  36.910  1.00  9.22           C
ATOM    142  OG  SER A 397       5.712   8.496  37.719  1.00  6.50           O
ATOM    143  C   SER A 397       4.341  10.829  37.393  1.00 10.78           C
ATOM    144  O   SER A 397       5.208  11.660  37.349  1.00 10.33           O
ATOM    145  N   GLU A 398       3.475  10.725  38.380  1.00 12.24           N
ATOM    146  CA  GLU A 398       3.529  11.583  39.523  1.00 15.01           C
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ATOM    147  CB  GLU A 398       2.442  11.150  40.497  1.00 16.05           C
ATOM    148  CG  GLU A 398       1.144  10.725  39.763  1.00 22.93           C
ATOM    149  CD  GLU A 398       0.312  11.914  39.223  1.00 30.62           C
ATOM    150  OE1 GLU A 398      -0.005  12.877  40.018  1.00 28.54           O
ATOM    151  OE2 GLU A 398      -0.016  11.876  37.984  1.00 34.64           O
ATOM    152  C   GLU A 398       4.906  11.482  40.171  1.00 14.63           C
ATOM    153  O   GLU A 398       5.503  12.440  40.559  1.00 14.38           O
ATOM    154  N   ASN A 399       5.422  10.286  40.251  1.00 15.36           N
ATOM    155  CA  ASN A 399       6.715  10.093  40.828  1.00 15.54           C
ATOM    156  CB  ASN A 399       6.949   8.607  40.993  1.00 17.66           C
ATOM    157  CG  ASN A 399       7.545   8.279  42.313  1.00 23.36           C
ATOM    158  OD1 ASN A 399       8.739   8.543  42.555  1.00 29.18           O
ATOM    159  ND2 ASN A 399       6.719   7.744  43.213  1.00 26.01           N
ATOM    160  C   ASN A 399       7.843  10.673  40.001  1.00 14.48           C
ATOM    161  O   ASN A 399       8.811  11.219  40.573  1.00 14.83           O
ATOM    162  N   LEU A 400       7.747  10.584  38.663  1.00 11.35           N
ATOM    163  CA  LEU A 400       8.829  11.137  37.861  1.00  9.12           C
ATOM    164  CB  LEU A 400       8.722  10.696  36.425  1.00  8.94           C
ATOM    165  CG  LEU A 400       9.965  10.282  35.637  1.00  7.91           C
ATOM    166  CD1 LEU A 400       9.655  10.352  34.107  1.00  6.48           C
ATOM    167  CD2 LEU A 400      11.217  11.040  35.988  1.00  6.99           C
ATOM    168  C   LEU A 400       8.933  12.675  37.981  1.00  7.77           C
ATOM    169  O   LEU A 400      10.029  13.239  38.047  1.00  7.08           O
ATOM    170  N   ILE A 401       7.783  13.331  38.001  1.00  7.02           N
ATOM    171  CA  ILE A 401       7.672  14.766  38.198  1.00  6.74           C
ATOM    172  CB  ILE A 401       6.182  15.161  38.154  1.00  6.15           C
ATOM    173  CG1 ILE A 401       5.669  15.045  36.732  1.00  7.60           C
ATOM    174  CD1 ILE A 401       6.360  16.024  35.724  1.00  6.89           C
ATOM    175  CG2 ILE A 401       5.968  16.588  38.665  1.00  4.00           C
ATOM    176  C   ILE A 401       8.255  15.091  39.588  1.00  7.08           C
ATOM    177  O   ILE A 401       8.872  16.141  39.834  1.00  6.41           O
ATOM    178  N   SER A 402       8.112  14.141  40.479  1.00  6.89           N
ATOM    179  CA  SER A 402       8.660  14.353  41.773  1.00  9.50           C
ATOM    180  CB  SER A 402       8.347  13.166  42.680  1.00 10.22           C
ATOM    181  OG  SER A 402       9.222  13.157  43.782  1.00 14.32           O
ATOM    182  C   SER A 402      10.145  14.607  41.604  1.00  8.81           C
ATOM    183  O   SER A 402      10.687  15.584  42.107  1.00  8.60           O
ATOM    184  N   TYR A 403      10.799  13.744  40.852  1.00  9.20           N
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ATOM    185  CA  TYR A 403      12.231  13.941  40.585  1.00  9.67           C
ATOM    186  CB  TYR A 403      12.780  12.753  39.816  1.00  9.50           C
ATOM    187  CG  TYR A 403      13.035  11.498  40.641  1.00 10.54           C
ATOM    188  CD1 TYR A 403      14.106  11.434  41.555  1.00 11.31           C
ATOM    189  CE1 TYR A 403      14.355  10.307  42.276  1.00  9.55           C
ATOM    190  CZ  TYR A 403      13.546   9.194  42.063  1.00 10.21           C
ATOM    191  OH  TYR A 403      13.807   8.017  42.705  1.00 12.21           O
ATOM    192  CE2 TYR A 403      12.514   9.224  41.171  1.00  6.97           C
ATOM    193  CD2 TYR A 403      12.251  10.368  40.475  1.00  7.64           C
ATOM    194  C   TYR A 403      12.579  15.264  39.824  1.00  9.18           C
ATOM    195  O   TYR A 403      13.591  15.916  40.165  1.00  8.20           O
ATOM    196  N   PHE A 404      11.751  15.634  38.836  1.00  7.17           N
ATOM    197  CA  PHE A 404      11.953  16.876  38.133  1.00  8.77           C
ATOM    198  CB  PHE A 404      10.904  17.114  36.997  1.00  9.18           C
ATOM    199  CG  PHE A 404      10.887  16.043  35.902  1.00  6.14           C
ATOM    200  CD1 PHE A 404      11.894  15.068  35.828  1.00  4.71           C
ATOM    201  CE1 PHE A 404      11.866  14.087  34.869  1.00  2.70           C
ATOM    202  CZ  PHE A 404      10.849  14.068  33.889  1.00  2.00           C
ATOM    203  CE2 PHE A 404       9.856  15.048  33.939  1.00  2.00           C
ATOM    204  CD2 PHE A 404       9.876  16.016  34.964  1.00  2.00           C
ATOM    205  C   PHE A 404      11.909  18.081  39.104  1.00 10.04           C
ATOM    206  O   PHE A 404      12.696  19.011  38.979  1.00 10.48           O
ATOM    207  N   ASN A 405      10.991  18.073  40.060  1.00 10.29           N
ATOM    208  CA  ASN A 405      10.927  19.164  41.005  1.00 11.87           C
ATOM    209  CB  ASN A 405       9.546  19.150  41.687  1.00 13.31           C
ATOM    210  CG  ASN A 405       8.446  19.650  40.757  1.00 14.99           C
ATOM    211  OD1 ASN A 405       7.272  19.493  41.026  1.00 18.52           O
ATOM    212  ND2 ASN A 405       8.844  20.265  39.670  1.00 12.65           N
ATOM    213  C   ASN A 405      12.056  19.165  42.080  1.00 11.91           C
ATOM    214  O   ASN A 405      12.255  20.149  42.813  1.00 10.19           O
ATOM    215  N   ASN A 406      12.779  18.060  42.188  1.00 11.31           N
ATOM    216  CA  ASN A 406      13.861  18.036  43.158  1.00 12.26           C
ATOM    217  CB  ASN A 406      14.059  16.626  43.708  1.00 12.84           C
ATOM    218  CG  ASN A 406      12.832  16.115  44.505  1.00 15.33           C
ATOM    219  OD1 ASN A 406      12.327  16.823  45.337  1.00 18.94           O
ATOM    220  ND2 ASN A 406      12.371  14.902  44.231  1.00 16.26           N
ATOM    221  C   ASN A 406      15.190  18.520  42.617  1.00 12.01           C
ATOM    222  O   ASN A 406      16.155  18.526  43.373  1.00 13.01           O
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ATOM    223  N   CYS A 407      15.245  18.845  41.316  1.00 10.65           N
ATOM    224  CA  CYS A 407      16.454  19.284  40.629  1.00  9.58           C
ATOM    225  CB  CYS A 407      16.358  19.051  39.114  1.00  9.61           C
ATOM    226  SG  CYS A 407      16.101  17.366  38.388  1.00  7.04           S
ATOM    227  C   CYS A 407      16.871  20.772  40.900  1.00  9.92           C
ATOM    228  O   CYS A 407      16.056  21.660  41.100  1.00 10.76           O
ATOM    229  N   THR A 408      18.163  21.036  40.929  1.00  9.20           N
ATOM    230  CA  THR A 408      18.625  22.387  41.057  1.00  8.76           C
ATOM    231  CB  THR A 408      20.132  22.403  40.955  1.00  9.46           C
ATOM    232  OG1 THR A 408      20.746  21.698  42.061  1.00 10.38           O
ATOM    233  CG2 THR A 408      20.691  23.859  41.004  1.00  8.49           C
ATOM    234  C   THR A 408      18.050  23.190  39.890  1.00  8.65           C
ATOM    235  O   THR A 408      17.807  24.356  40.027  1.00  9.13           O
ATOM    236  N   VAL A 409      17.892  22.573  38.723  1.00  8.51           N
ATOM    237  CA  VAL A 409      17.326  23.248  37.583  1.00  7.79           C
ATOM    238  CB  VAL A 409      18.360  23.399  36.466  1.00  8.28           C
ATOM    239  CG1 VAL A 409      17.817  24.215  35.268  1.00  6.45           C
ATOM    240  CG2 VAL A 409      19.606  23.974  36.989  1.00  7.43           C
ATOM    241  C   VAL A 409      16.213  22.344  37.104  1.00  8.17           C
ATOM    242  O   VAL A 409      16.457  21.179  36.907  1.00  7.93           O
ATOM    243  N   ASN A 410      15.007  22.876  36.914  1.00  7.49           N
ATOM    244  CA  ASN A 410      13.864  22.062  36.530  1.00  8.42           C
ATOM    245  CB  ASN A 410      12.566  22.786  36.929  1.00  8.29           C
ATOM    246  CG  ASN A 410      11.361  21.860  36.935  1.00  7.78           C
ATOM    247  OD1 ASN A 410      11.027  21.254  35.930  1.00 17.24           O
ATOM    248  ND2 ASN A 410      10.706  21.767  38.037  1.00  2.36           N
ATOM    249  C   ASN A 410      13.835  21.629  35.028  1.00  8.35           C
ATOM    250  O   ASN A 410      13.852  22.453  34.141  1.00  7.62           O
ATOM    251  N   PRO A 411      13.848  20.329  34.765  1.00  8.01           N
ATOM    252  CA  PRO A 411      13.819  19.811  33.385  1.00  7.91           C
ATOM    253  CB  PRO A 411      14.685  18.525  33.482  1.00  6.94           C
ATOM    254  CG  PRO A 411      14.357  17.998  34.864  1.00  6.32           C
ATOM    255  CD  PRO A 411      14.113  19.259  35.756  1.00  7.63           C
ATOM    256  C   PRO A 411      12.470  19.497  32.786  1.00  8.05           C
ATOM    257  O   PRO A 411      12.384  19.310  31.569  1.00  9.08           O
ATOM    258  N   LYS A 412      11.422  19.458  33.581  1.00  8.49           N
ATOM    259  CA  LYS A 412      10.086  19.154  33.046  1.00  9.75           C
ATOM    260  CB  LYS A 412       9.052  19.504  34.066  1.00  9.19           C
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ATOM    261  CG  LYS A 412       7.744  18.856  33.805  1.00 12.96           C
ATOM    262  CD  LYS A 412       6.730  19.221  34.859  1.00 20.30           C
ATOM    263  CE  LYS A 412       5.921  20.478  34.478  1.00 22.28           C
ATOM    264  NZ  LYS A 412       4.874  20.156  33.455  1.00 24.30           N
ATOM    265  C   LYS A 412       9.717  19.867  31.717  1.00 10.16           C
ATOM    266  O   LYS A 412       8.997  19.336  30.884  1.00  9.72           O
ATOM    267  N   GLU A 413      10.253  21.055  31.526  1.00 10.93           N
ATOM    268  CA  GLU A 413       9.971  21.858  30.354  1.00 12.98           C
ATOM    269  CB  GLU A 413      10.335  23.314  30.655  1.00 14.77           C
ATOM    270  CG  GLU A 413       9.876  24.252  29.569  1.00 22.12           C
ATOM    271  CD  GLU A 413       8.366  24.221  29.395  1.00 30.57           C
ATOM    272  OE1 GLU A 413       7.756  23.307  30.039  1.00 29.00           O
ATOM    273  OE2 GLU A 413       7.827  25.111  28.609  1.00 33.99           O
ATOM    274  C   GLU A 413      10.693  21.398  29.080  1.00 10.78           C
ATOM    275  O   GLU A 413      10.082  21.129  28.015  1.00 10.26           O
ATOM    276  N   SER A 414      12.000  21.334  29.166  1.00  8.08           N
ATOM    277  CA  SER A 414      12.715  20.831  28.041  1.00  6.45           C
ATOM    278  CB  SER A 414      14.174  20.915  28.308  1.00  5.87           C
ATOM    279  OG  SER A 414      14.513  22.221  28.671  1.00  6.24           O
ATOM    280  C   SER A 414      12.315  19.363  27.800  1.00  6.66           C
ATOM    281  O   SER A 414      12.313  18.909  26.691  1.00  6.05           O
ATOM    282  N   ILE A 415      11.998  18.602  28.836  1.00  7.08           N
ATOM    283  CA  ILE A 415      11.537  17.282  28.494  1.00  9.05           C
ATOM    284  CB  ILE A 415      11.925  16.069  29.384  1.00  8.83           C
ATOM    285  CG1 ILE A 415      13.023  16.338  30.443  1.00  5.60           C
ATOM    286  CD1 ILE A 415      13.107  15.477  31.689  1.00  2.00           C
ATOM    287  CG2 ILE A 415      12.878  15.445  28.216  1.00 17.75           C
ATOM    288  C   ILE A 415      10.274  17.026  27.672  1.00  8.74           C
ATOM    289  O   ILE A 415      10.253  16.110  26.813  1.00  7.52           O
ATOM    290  N   LEU A 416       9.241  17.788  27.974  1.00  7.71           N
ATOM    291  CA  LEU A 416       8.015  17.661  27.301  1.00  7.92           C
ATOM    292  CB  LEU A 416       6.969  18.514  28.017  1.00  7.90           C
ATOM    293  CG  LEU A 416       6.634  18.055  29.452  1.00 11.36           C
ATOM    294  CD1 LEU A 416       5.682  19.021  30.228  1.00 11.42           C
ATOM    295  CD2 LEU A 416       6.048  16.647  29.484  1.00  3.28           C
ATOM    296  C   LEU A 416       8.200  18.184  25.872  1.00  7.77           C
ATOM    297  O   LEU A 416       7.621  17.588  24.900  1.00  8.01           O
ATOM    298  N   LYS A 417       8.960  19.286  25.732  1.00  5.60           N
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ATOM    299  CA  LYS A 417       9.069  19.937  24.417  1.00  4.70           C
ATOM    300  CB  LYS A 417       9.624  21.362  24.537  1.00  6.05           C
ATOM    301  CG  LYS A 417       8.714  22.296  25.374  1.00  7.81           C
ATOM    302  CD  LYS A 417       9.342  23.738  25.642  1.00 10.54           C
ATOM    303  CE  LYS A 417       9.498  24.562  24.365  1.00  9.12           C
ATOM    304  NZ  LYS A 417       8.200  24.843  23.770  1.00  5.02           N
ATOM    305  C   LYS A 417       9.864  19.111  23.462  1.00  3.25           C
ATOM    306  O   LYS A 417       9.522  18.992  22.249  1.00  2.53           O
ATOM    307  N   ARG A 418      10.838  18.424  24.027  1.00  2.00           N
ATOM    308  CA  ARG A 418      11.675  17.530  23.239  1.00  2.82           C
ATOM    309  CB  ARG A 418      12.913  17.084  24.007  1.00  2.07           C
ATOM    310  CG  ARG A 418      13.990  16.222  23.291  1.00  3.70           C
ATOM    311  CD  ARG A 418      15.353  16.381  23.949  1.00  3.44           C
ATOM    312  NE  ARG A 418      15.052  16.283  25.337  1.00  9.38           N
ATOM    313  CZ  ARG A 418      15.626  16.901  26.313  1.00  6.00           C
ATOM    314  NH1 ARG A 418      16.644  17.717  26.110  1.00  9.43           N
ATOM    315  NH2 ARG A 418      15.149  16.666  27.520  1.00  7.51           N
ATOM    316  C   ARG A 418      10.873  16.374  22.687  1.00  3.56           C
ATOM    317  O   ARG A 418      11.026  16.045  21.472  1.00  3.39           O
ATOM    318  N   VAL A 419      10.022  15.771  23.546  1.00  2.74           N
ATOM    319  CA  VAL A 419       9.148  14.671  23.100  1.00  2.74           C
ATOM    320  CB  VAL A 419       8.360  14.001  24.269  1.00  3.32           C
ATOM    321  CG1 VAL A 419       7.306  13.052  23.758  1.00  2.00           C
ATOM    322  CG2 VAL A 419       9.276  13.300  25.281  1.00  3.25           C
ATOM    323  C   VAL A 419       8.193  15.168  21.994  1.00  2.42           C
ATOM    324  O   VAL A 419       8.034  14.535  20.971  1.00  3.50           O
ATOM    325  N   LYS A 420       7.615  16.337  22.159  1.00  3.84           N
ATOM    326  CA  LYS A 420       6.751  16.936  21.135  1.00  6.62           C
ATOM    327  CB  LYS A 420       6.277  18.304  21.639  1.00  9.19           C
ATOM    328  CG  LYS A 420       4.764  18.548  21.803  1.00 12.82           C
ATOM    329  CD  LYS A 420       4.215  19.176  20.530  1.00 18.36           C
ATOM    330  CE  LYS A 420       4.359  18.239  19.264  1.00 22.97           C
ATOM    331  NZ  LYS A 420       4.073  18.902  17.861  1.00 14.81           N
ATOM    332  C   LYS A 420       7.452  17.114  19.771  1.00  6.45           C
ATOM    333  O   LYS A 420       6.947  16.694  18.733  1.00  5.83           O
ATOM    334  N   ASP A 421       8.638  17.722  19.772  1.00  7.00           N
ATOM    335  CA  ASP A 421       9.337  17.999  18.503  1.00  5.93           C
ATOM    336  CB  ASP A 421      10.454  19.038  18.683  1.00  5.34           C
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ATOM    337  CG  ASP A 421       9.935  20.397  19.244  1.00 10.31           C
ATOM    338  OD1 ASP A 421       8.673  20.653  19.288  1.00  6.28           O
ATOM    339  OD2 ASP A 421      10.768  21.259  19.696  1.00 14.34           O
ATOM    340  C   ASP A 421       9.890  16.750  17.838  1.00  5.07           C
ATOM    341  O   ASP A 421       9.683  16.527  16.652  1.00  6.86           O
ATOM    342  N   ILE A 422      10.620  15.923  18.552  1.00  3.56           N
ATOM    343  CA  ILE A 422      11.120  14.727  17.945  1.00  2.48           C
ATOM    344  CB  ILE A 422      11.830  13.913  18.957  1.00  2.93           C
ATOM    345  CG1 ILE A 422      13.031  14.638  19.545  1.00  2.54           C
ATOM    346  CD1 ILE A 422      13.975  15.166  18.435  1.00  5.66           C
ATOM    347  CG2 ILE A 422      12.172  12.511  18.367  1.00  2.78           C
ATOM    348  C   ILE A 422       9.931  13.895  17.402  1.00  2.68           C
ATOM    349  O   ILE A 422       9.990  13.371  16.355  1.00  2.00           O
ATOM    350  N   GLY A 423       8.834  13.746  18.125  1.00  3.53           N
ATOM    351  CA  GLY A 423       7.756  12.986  17.534  1.00  3.60           C
ATOM    352  C   GLY A 423       7.330  13.576  16.190  1.00  5.15           C
ATOM    353  O   GLY A 423       6.867  12.817  15.328  1.00  5.53           O
ATOM    354  N   TYR A 424       7.468  14.901  16.007  1.00  3.70           N
ATOM    355  CA  TYR A 424       6.999  15.558  14.812  1.00  4.56           C
ATOM    356  CB  TYR A 424       6.996  17.095  14.956  1.00  4.66           C
ATOM    357  CG  TYR A 424       6.643  17.772  13.661  1.00  2.59           C
ATOM    358  CD1 TYR A 424       5.339  17.825  13.223  1.00  2.76           C
ATOM    359  CE1 TYR A 424       5.024  18.381  12.022  1.00  3.68           C
ATOM    360  CZ  TYR A 424       5.981  18.940  11.251  1.00  5.36           C
ATOM    361  OH  TYR A 424       5.659  19.548  10.085  1.00 10.06           O
ATOM    362  CE2 TYR A 424       7.274  18.940  11.653  1.00  6.09           C
ATOM    363  CD2 TYR A 424       7.608  18.338  12.866  1.00  4.14           C
ATOM    364  C   TYR A 424       7.946  15.174  13.665  1.00  4.75           C
ATOM    365  O   TYR A 424       7.538  14.845  12.550  1.00  3.97           O
ATOM    366  N   ILE A 425       9.208  15.194  13.996  1.00  5.11           N
ATOM    367  CA  ILE A 425      10.246  14.814  13.086  1.00  6.31           C
ATOM    368  CB  ILE A 425      11.575  15.256  13.706  1.00  7.12           C
ATOM    369  CG1 ILE A 425      11.591  16.788  13.651  1.00  8.77           C
ATOM    370  CD1 ILE A 425      12.912  17.423  13.998  1.00 11.84           C
ATOM    371  CG2 ILE A 425      12.770  14.644  13.013  1.00  6.38           C
ATOM    372  C   ILE A 425      10.245  13.338  12.694  1.00  6.08           C
ATOM    373  O   ILE A 425      10.494  13.013  11.505  1.00  6.94           O
ATOM    374  N   PHE A 426       9.942  12.475  13.661  1.00  4.61           N
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ATOM	375	CA	PHE A 426	9.951	11.028	13.521	1.00	4.17	C
ATOM	376	CB	PHE A 426	9.753	10.393	14.915	1.00	3.43	C
ATOM	377	CG	PHE A 426	9.726	8.882	14.904	1.00	4.06	C
ATOM	378	CD1	PHE A 426	8.549	8.213	14.646	1.00	2.00	C
ATOM	379	CE1	PHE A 426	8.518	6.847	14.597	1.00	2.00	C
ATOM	380	CZ	PHE A 426	9.642	6.104	14.835	1.00	2.49	C
ATOM	381	CE2	PHE A 426	10.861	6.767	15.101	1.00	5.74	C
ATOM	382	CD2	PHE A 426	10.903	8.140	15.104	1.00	2.77	C
ATOM	383	C	PHE A 426	8.872	10.489	12.555	1.00	5.54	C
ATOM	384	O	PHE A 426	9.126	9.583	11.779	1.00	5.57	O
ATOM	385	N	LYS A 427	7.651	11.011	12.633	1.00	6.97	N
ATOM	386	CA	LYS A 427	6.582	10.546	11.739	1.00	7.52	C
ATOM	387	CB	LYS A 427	5.192	11.052	12.102	1.00	7.33	C
ATOM	388	CG	LYS A 427	4.705	10.664	13.535	1.00	13.06	C
ATOM	389	CD	LYS A 427	3.495	11.526	13.935	1.00	21.22	C
ATOM	390	CE	LYS A 427	3.309	11.580	15.408	1.00	28.07	C
ATOM	391	NZ	LYS A 427	4.036	12.688	16.156	1.00	28.68	N
ATOM	392	C	LYS A 427	6.880	10.870	10.317	1.00	5.90	C
ATOM	393	O	LYS A 427	6.715	10.025	9.441	1.00	6.60	O
ATOM	394	N	GLU A 428	7.364	12.069	10.081	1.00	5.34	N
ATOM	395	CA	GLU A 428	7.608	12.462	8.709	1.00	5.59	C
ATOM	396	CB	GLU A 428	7.930	13.958	8.614	1.00	5.72	C
ATOM	397	CG	GLU A 428	6.890	14.894	9.187	1.00	6.84	C
ATOM	398	CD	GLU A 428	5.572	14.861	8.439	1.00	12.45	C
ATOM	399	OE1	GLU A 428	5.630	14.955	7.186	1.00	19.41	O
ATOM	400	OE2	GLU A 428	4.475	14.734	9.075	1.00	8.62	O
ATOM	401	C	GLU A 428	8.720	11.563	8.091	1.00	4.41	C
ATOM	402	O	GLU A 428	8.634	11.081	6.969	1.00	3.48	O
ATOM	403	N	LYS A 429	9.745	11.339	8.883	1.00	4.31	N
ATOM	404	CA	LYS A 429	10.831	10.497	8.509	1.00	4.32	C
ATOM	405	CB	LYS A 429	11.939	10.610	9.514	1.00	4.54	C
ATOM	406	CG	LYS A 429	12.655	11.990	9.432	1.00	5.96	C
ATOM	407	CD	LYS A 429	14.004	12.046	10.143	1.00	5.92	C
ATOM	408	CE	LYS A 429	14.709	13.432	9.940	1.00	5.19	C
ATOM	409	NZ	LYS A 429	16.072	13.456	10.579	1.00	3.04	N
ATOM	410	C	LYS A 429	10.404	9.085	8.301	1.00	4.70	C
ATOM	411	O	LYS A 429	10.740	8.458	7.295	1.00	3.93	O
ATOM	412	N	PHE A 430	9.557	8.607	9.197	1.00	6.56	N

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ATOM    413  CA  PHE A 430       9.124   7.229   9.124  1.00  7.38           C
ATOM    414  CB  PHE A 430       8.236   6.911  10.323  1.00  7.54           C
ATOM    415  CG  PHE A 430       7.907   5.450  10.464  1.00  8.61           C
ATOM    416  CD1 PHE A 430       7.066   4.830   9.564  1.00 11.42           C
ATOM    417  CE1 PHE A 430       6.769   3.531   9.687  1.00 12.86           C
ATOM    418  CZ  PHE A 430       7.329   2.825  10.689  1.00 13.90           C
ATOM    419  CE2 PHE A 430       8.207   3.404  11.558  1.00  9.63           C
ATOM    420  CD2 PHE A 430       8.469   4.699  11.469  1.00  7.48           C
ATOM    421  C   PHE A 430       8.411   7.061   7.772  1.00  7.72           C
ATOM    422  O   PHE A 430       8.846   6.303   6.897  1.00  6.61           O
ATOM    423  N   ALA A 431       7.334   7.807   7.602  1.00  8.28           N
ATOM    424  CA  ALA A 431       6.583   7.787   6.355  1.00 10.41           C
ATOM    425  CB  ALA A 431       5.660   8.974   6.307  1.00  9.96           C
ATOM    426  C   ALA A 431       7.482   7.834   5.109  1.00 13.02           C
ATOM    427  O   ALA A 431       7.248   7.119   4.125  1.00 11.76           O
ATOM    428  N   LYS A 432       8.494   8.710   5.142  1.00 15.88           N
ATOM    429  CA  LYS A 432       9.407   8.866   4.022  1.00 18.85           C
ATOM    430  CB  LYS A 432      10.328  10.025   4.327  1.00 20.32           C
ATOM    431  CG  LYS A 432      11.123  10.540   3.144  1.00 25.80           C
ATOM    432  CD  LYS A 432      12.118  11.692   3.537  1.00 32.56           C
ATOM    433  CE  LYS A 432      11.389  12.923   4.109  1.00 36.99           C
ATOM    434  NZ  LYS A 432      12.281  14.009   4.701  1.00 35.79           N
ATOM    435  C   LYS A 432      10.218   7.574   3.842  1.00 19.52           C
ATOM    436  O   LYS A 432      10.266   7.003   2.783  1.00 19.79           O
ATOM    437  N   ALA A 433      10.789   7.038   4.909  1.00 20.45           N
ATOM    438  CA  ALA A 433      11.573   5.818   4.747  1.00 20.25           C
ATOM    439  CB  ALA A 433      12.205   5.439   6.008  1.00 19.26           C
ATOM    440  C   ALA A 433      10.685   4.696   4.273  1.00 20.97           C
ATOM    441  O   ALA A 433      11.085   3.860   3.522  1.00 19.77           O
ATOM    442  N   VAL A 434       9.471   4.656   4.772  1.00 23.20           N
ATOM    443  CA  VAL A 434       8.589   3.571   4.450  1.00 24.82           C
ATOM    444  CB  VAL A 434       7.473   3.514   5.426  1.00 23.74           C
ATOM    445  CG1 VAL A 434       6.429   2.537   4.929  1.00 26.52           C
ATOM    446  CG2 VAL A 434       7.992   3.073   6.705  1.00 26.22           C
ATOM    447  C   VAL A 434       8.011   3.810   3.087  1.00 26.57           C
ATOM    448  O   VAL A 434       7.026   4.512   2.937  1.00 28.03           O
ATOM    449  N   GLY A 435       8.605   3.225   2.071  1.00 28.57           N
ATOM    450  CA  GLY A 435       8.073   3.426   0.753  1.00 30.76           C
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ATOM    451  C   GLY A 435       7.687   4.898   0.666  1.00 32.32           C
ATOM    452  O   GLY A 435       8.546   5.752   0.859  1.00 32.41           O
ATOM    453  N   GLN A 436       6.401   5.184   0.440  1.00 32.95           N
ATOM    454  CA  GLN A 436       5.958   6.530   0.236  1.00 34.18           C
ATOM    455  CB  GLN A 436       6.058   6.779  -1.265  1.00 35.09           C
ATOM    456  CG  GLN A 436       7.501   6.823  -1.799  1.00 38.55           C
ATOM    457  CD  GLN A 436       7.698   6.064  -3.115  1.00 40.82           C
ATOM    458  OE1 GLN A 436       8.670   6.317  -3.836  1.00 42.49           O
ATOM    459  NE2 GLN A 436       6.778   5.145  -3.431  1.00 41.77           N
ATOM    460  C   GLN A 436       4.522   6.874   0.738  1.00 34.26           C
ATOM    461  O   GLN A 436       3.675   5.955   0.911  1.00 34.87           O
ATOM    462  N   GLY A 437       4.278   8.185   0.952  1.00 32.88           N
ATOM    463  CA  GLY A 437       2.979   8.731   1.293  1.00 32.07           C
ATOM    464  C   GLY A 437       2.649   9.129   2.729  1.00 31.84           C
ATOM    465  O   GLY A 437       3.329   9.947   3.330  1.00 33.28           O
ATOM    466  N   CYS A 438       1.569   8.559   3.264  1.00 30.09           N
ATOM    467  CA  CYS A 438       1.081   8.811   4.618  1.00 28.02           C
ATOM    468  CB  CYS A 438      -0.349   9.405   4.591  1.00 28.75           C
ATOM    469  SG  CYS A 438      -1.524   8.660   5.796  1.00 30.36           S
ATOM    470  C   CYS A 438       1.019   7.448   5.270  1.00 26.25           C
ATOM    471  O   CYS A 438       0.383   6.535   4.724  1.00 24.75           O
ATOM    472  N   VAL A 439       1.680   7.320   6.426  1.00 24.37           N
ATOM    473  CA  VAL A 439       1.801   6.035   7.132  1.00 22.64           C
ATOM    474  CB  VAL A 439       3.252   5.510   7.079  1.00 22.72           C
ATOM    475  CG1 VAL A 439       3.330   4.007   7.496  1.00 22.50           C
ATOM    476  CG2 VAL A 439       3.826   5.722   5.695  1.00 22.13           C
ATOM    477  C   VAL A 439       1.303   6.064   8.591  1.00 21.76           C
ATOM    478  O   VAL A 439       2.080   6.166   9.531  1.00 18.79           O
ATOM    479  N   GLU A 440      -0.016   5.952   8.749  1.00 21.55           N
ATOM    480  CA  GLU A 440      -0.623   5.986  10.061  1.00 21.30           C
ATOM    481  CB  GLU A 440      -2.104   5.639   9.974  1.00 22.04           C
ATOM    482  CG  GLU A 440      -2.941   6.602   9.153  1.00 23.35           C
ATOM    483  CD  GLU A 440      -4.398   6.142   9.025  1.00 27.57           C
ATOM    484  OE1 GLU A 440      -4.964   5.665  10.046  1.00 29.99           O
ATOM    485  OE2 GLU A 440      -5.002   6.237   7.914  1.00 27.95           O
ATOM    486  C   GLU A 440       0.081   5.115  11.119  1.00 20.38           C
ATOM    487  O   GLU A 440      -0.247   5.193  12.283  1.00 21.06           O
ATOM    488  N   ILE A 441       1.098   4.348  10.760  1.00 19.36           N
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ATOM    489  CA  ILE A 441       1.691   3.450  11.758  1.00 18.24           C
ATOM    490  CB  ILE A 441       2.085   2.105  11.088  1.00 18.75           C
ATOM    491  CG1 ILE A 441       0.893   1.146  11.125  1.00 21.67           C
ATOM    492  CD1 ILE A 441      -0.283   1.567  10.160  1.00 26.94           C
ATOM    493  CG2 ILE A 441       3.147   1.404  11.844  1.00 22.00           C
ATOM    494  C   ILE A 441       2.832   4.072  12.555  1.00 16.39           C
ATOM    495  O   ILE A 441       3.166   3.652  13.665  1.00 15.75           O
ATOM    496  N   GLY A 442       3.440   5.089  11.968  1.00 14.93           N
ATOM    497  CA  GLY A 442       4.514   5.798  12.581  1.00 13.46           C
ATOM    498  C   GLY A 442       4.109   6.399  13.897  1.00 14.00           C
ATOM    499  O   GLY A 442       4.862   6.323  14.833  1.00 16.06           O
ATOM    500  N   SER A 443       2.940   7.002  13.990  1.00 13.14           N
ATOM    501  CA  SER A 443       2.463   7.538  15.243  1.00 12.84           C
ATOM    502  CB  SER A 443       1.049   8.104  15.060  1.00 12.90           C
ATOM    503  OG  SER A 443       1.074   9.243  14.212  1.00 17.50           O
ATOM    504  C   SER A 443       2.366   6.520  16.346  1.00 12.40           C
ATOM    505  O   SER A 443       2.867   6.744  17.417  1.00 12.76           O
ATOM    506  N   GLN A 444       1.694   5.409  16.075  1.00 12.47           N
ATOM    507  CA  GLN A 444       1.407   4.381  17.069  1.00 12.70           C
ATOM    508  CB  GLN A 444       0.527   3.245  16.467  1.00 12.40           C
ATOM    509  CG  GLN A 444       0.280   1.987  17.407  1.00 17.53           C
ATOM    510  CD  GLN A 444      -1.153   1.909  18.097  1.00 20.42           C
ATOM    511  OE1 GLN A 444      -1.419   2.577  19.145  1.00 19.65           O
ATOM    512  NE2 GLN A 444      -2.048   1.106  17.506  1.00 16.04           N
ATOM    513  C   GLN A 444       2.729   3.893  17.660  1.00 11.87           C
ATOM    514  O   GLN A 444       2.833   3.634  18.875  1.00 10.62           O
ATOM    515  N   ARG A 445       3.765   3.836  16.821  1.00 10.93           N
ATOM    516  CA  ARG A 445       5.022   3.341  17.337  1.00 10.57           C
ATOM    517  CB  ARG A 445       5.910   2.901  16.201  1.00 12.33           C
ATOM    518  CG  ARG A 445       5.318   1.798  15.401  1.00 15.05           C
ATOM    519  CD  ARG A 445       6.277   1.028  14.668  1.00 20.23           C
ATOM    520  NE  ARG A 445       5.592   0.089  13.790  1.00 27.54           N
ATOM    521  CZ  ARG A 445       6.170  -0.577  12.776  1.00 29.64           C
ATOM    522  NH1 ARG A 445       7.471  -0.444  12.508  1.00 26.97           N
ATOM    523  NH2 ARG A 445       5.432  -1.411  12.047  1.00 32.65           N
ATOM    524  C   ARG A 445       5.751   4.342  18.236  1.00  9.95           C
ATOM    525  O   ARG A 445       6.220   3.973  19.354  1.00  9.16           O
ATOM    526  N   TYR A 446       5.860   5.593  17.764  1.00  7.68           N
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ATOM    527  CA  TYR A 446       6.505   6.634  18.558  1.00  6.37           C
ATOM    528  CB  TYR A 446       6.448   7.988  17.835  1.00  6.60           C
ATOM    529  CG  TYR A 446       7.190   9.082  18.575  1.00  3.78           C
ATOM    530  CD1 TYR A 446       8.564   9.103  18.559  1.00  2.15           C
ATOM    531  CE1 TYR A 446       9.264  10.019  19.243  1.00  2.00           C
ATOM    532  CZ  TYR A 446       8.646  10.974  19.966  1.00  2.00           C
ATOM    533  OH  TYR A 446       9.472  11.916  20.558  1.00  2.42           O
ATOM    534  CE2 TYR A 446       7.293  11.020  20.022  1.00  2.00           C
ATOM    535  CD2 TYR A 446       6.533  10.064  19.311  1.00  2.00           C
ATOM    536  C   TYR A 446       5.895   6.730  19.983  1.00  5.32           C
ATOM    537  O   TYR A 446       6.611   6.820  20.978  1.00  3.64           O
ATOM    538  N   LYS A 447       4.568   6.669  20.054  1.00  3.91           N
ATOM    539  CA  LYS A 447       3.856   6.656  21.333  1.00  3.14           C
ATOM    540  CB  LYS A 447       2.336   6.580  21.139  1.00  2.11           C
ATOM    541  CG  LYS A 447       1.767   7.958  20.756  1.00  4.83           C
ATOM    542  CD  LYS A 447       0.326   7.986  20.456  1.00 12.30           C
ATOM    543  CE  LYS A 447      -0.122   9.423  19.935  1.00 19.61           C
ATOM    544  NZ  LYS A 447       0.615   9.946  18.721  1.00 25.13           N
ATOM    545  C   LYS A 447       4.301   5.563  22.287  1.00  3.08           C
ATOM    546  O   LYS A 447       4.442   5.807  23.476  1.00  2.00           O
ATOM    547  N   LEU A 448       4.487   4.354  21.742  1.00  3.95           N
ATOM    548  CA  LEU A 448       4.899   3.219  22.509  1.00  3.91           C
ATOM    549  CB  LEU A 448       4.829   1.917  21.677  1.00  4.54           C
ATOM    550  CG  LEU A 448       3.444   1.290  21.488  1.00  6.42           C
ATOM    551  CD1 LEU A 448       3.498   0.126  20.480  1.00  4.90           C
ATOM    552  CD2 LEU A 448       2.885   0.833  22.829  1.00  2.56           C
ATOM    553  C   LEU A 448       6.327   3.501  22.949  1.00  3.00           C
ATOM    554  O   LEU A 448       6.724   3.194  24.097  1.00  2.00           O
ATOM    555  N   GLY A 449       7.089   4.088  22.029  1.00  2.24           N
ATOM    556  CA  GLY A 449       8.440   4.523  22.383  1.00  3.49           C
ATOM    557  C   GLY A 449       8.432   5.426  23.628  1.00  4.47           C
ATOM    558  O   GLY A 449       9.127   5.100  24.600  1.00  5.55           O
ATOM    559  N   VAL A 450       7.586   6.473  23.665  1.00  3.49           N
ATOM    560  CA  VAL A 450       7.575   7.363  24.792  1.00  4.55           C
ATOM    561  CB  VAL A 450       6.399   8.319  24.875  1.00  6.58           C
ATOM    562  CG1 VAL A 450       6.709   9.670  25.552  1.00  7.93           C
ATOM    563  CG2 VAL A 450       5.813   8.538  23.636  1.00 13.08           C
ATOM    564  C   VAL A 450       7.157   6.676  26.043  1.00  3.61           C
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ATOM    565  O   VAL A 450       7.611   7.058  27.139  1.00  2.67           O
ATOM    566  N   ARG A 451       6.181   5.784  25.926  1.00  2.00           N
ATOM    567  CA  ARG A 451       5.688   5.160  27.117  1.00  2.00           C
ATOM    568  CB  ARG A 451       4.415   4.350  26.864  1.00  2.00           C
ATOM    569  CG  ARG A 451       3.265   5.172  26.369  1.00  2.00           C
ATOM    570  CD  ARG A 451       2.114   4.324  25.965  1.00  5.40           C
ATOM    571  NE  ARG A 451       0.956   5.069  25.455  1.00 10.15           N
ATOM    572  CZ  ARG A 451      -0.248   4.474  25.274  1.00 14.62           C
ATOM    573  NH1 ARG A 451      -0.364   3.167  25.570  1.00 13.39           N
ATOM    574  NH2 ARG A 451      -1.326   5.159  24.828  1.00 11.66           N
ATOM    575  C   ARG A 451       6.801   4.316  27.772  1.00  2.00           C
ATOM    576  O   ARG A 451       6.862   4.221  28.985  1.00  2.06           O
ATOM    577  N   LEU A 452       7.694   3.779  26.968  1.00  2.00           N
ATOM    578  CA  LEU A 452       8.787   2.978  27.445  1.00  2.00           C
ATOM    579  CB  LEU A 452       9.493   2.241  26.276  1.00  2.00           C
ATOM    580  CG  LEU A 452       9.745   0.778  26.453  1.00  3.02           C
ATOM    581  CD1 LEU A 452      10.674   0.419  25.328  1.00  5.79           C
ATOM    582  CD2 LEU A 452      10.172   0.204  27.937  1.00  2.00           C
ATOM    583  C   LEU A 452       9.821   3.895  28.051  1.00  2.00           C
ATOM    584  O   LEU A 452      10.339   3.642  29.139  1.00  2.00           O
ATOM    585  N   TYR A 453      10.108   4.944  27.287  1.00  2.78           N
ATOM    586  CA  TYR A 453      11.061   6.011  27.640  1.00  3.85           C
ATOM    587  CB  TYR A 453      10.910   7.176  26.662  1.00  3.22           C
ATOM    588  CG  TYR A 453      11.501   8.535  27.070  1.00  2.74           C
ATOM    589  CD1 TYR A 453      12.868   8.741  27.164  1.00  2.00           C
ATOM    590  CE1 TYR A 453      13.402   9.990  27.425  1.00  2.00           C
ATOM    591  CZ  TYR A 453      12.543  11.062  27.581  1.00  2.98           C
ATOM    592  OH  TYR A 453      12.996  12.386  27.820  1.00  2.14           O
ATOM    593  CE2 TYR A 453      11.177  10.869  27.486  1.00  2.00           C
ATOM    594  CD2 TYR A 453      10.675   9.642  27.209  1.00  2.00           C
ATOM    595  C   TYR A 453      10.847   6.521  29.061  1.00  2.90           C
ATOM    596  O   TYR A 453      11.761   6.551  29.867  1.00  2.00           O
ATOM    597  N   TYR A 454       9.603   6.875  29.346  1.00  2.73           N
ATOM    598  CA  TYR A 454       9.261   7.371  30.661  1.00  2.78           C
ATOM    599  CB  TYR A 454       7.886   8.025  30.665  1.00  2.00           C
ATOM    600  CG  TYR A 454       7.875   9.427  30.084  1.00  2.00           C
ATOM    601  CD1 TYR A 454       8.920  10.320  30.330  1.00  5.16           C
ATOM    602  CE1 TYR A 454       8.888  11.674  29.835  1.00  2.49           C
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ATOM    603  CZ  TYR A 454       7.841  12.047  29.107  1.00  2.99           C
ATOM    604  OH  TYR A 454       7.794  13.303  28.578  1.00  3.52           O
ATOM    605  CE2 TYR A 454       6.795  11.146  28.853  1.00  4.23           C
ATOM    606  CD2 TYR A 454       6.842   9.862  29.328  1.00  2.00           C
ATOM    607  C   TYR A 454       9.367   6.274  31.709  1.00  3.50           C
ATOM    608  O   TYR A 454       9.906   6.509  32.803  1.00  4.53           O
ATOM    609  N   ARG A 455       8.870   5.080  31.388  1.00  3.34           N
ATOM    610  CA  ARG A 455       8.891   3.972  32.323  1.00  3.12           C
ATOM    611  CB  ARG A 455       8.101   2.818  31.725  1.00  3.07           C
ATOM    612  CG  ARG A 455       8.180   1.507  32.471  1.00  2.58           C
ATOM    613  CD  ARG A 455       7.680   0.344  31.669  1.00  2.00           C
ATOM    614  NE  ARG A 455       8.236  -0.942  32.090  1.00  6.42           N
ATOM    615  CZ  ARG A 455       7.807  -1.662  33.179  1.00 11.99           C
ATOM    616  NH1 ARG A 455       8.348  -2.862  33.469  1.00  9.20           N
ATOM    617  NH2 ARG A 455       6.802  -1.218  33.939  1.00  9.54           N
ATOM    618  C   ARG A 455      10.365   3.589  32.710  1.00  4.18           C
ATOM    619  O   ARG A 455      10.681   3.275  33.841  1.00  5.50           O
ATOM    620  N   VAL A 456      11.282   3.706  31.771  1.00  4.54           N
ATOM    621  CA  VAL A 456      12.683   3.420  31.981  1.00  2.65           C
ATOM    622  CB  VAL A 456      13.312   3.113  30.643  1.00  2.00           C
ATOM    623  CG1 VAL A 456      14.859   3.065  30.755  1.00  4.98           C
ATOM    624  CG2 VAL A 456      12.742   1.787  30.107  1.00  2.00           C
ATOM    625  C   VAL A 456      13.432   4.511  32.717  1.00  2.66           C
ATOM    626  O   VAL A 456      14.296   4.238  33.552  1.00  3.62           O
ATOM    627  N   MET A 457      13.107   5.760  32.430  1.00  3.27           N
ATOM    628  CA  MET A 457      13.752   6.909  33.073  1.00  2.00           C
ATOM    629  CB  MET A 457      13.250   8.218  32.443  1.00  2.00           C
ATOM    630  CG  MET A 457      13.849   9.459  33.049  1.00  2.00           C
ATOM    631  SD  MET A 457      13.120  11.027  32.572  1.00  2.00           S
ATOM    632  CE  MET A 457      13.434  10.941  30.705  1.00  2.00           C
ATOM    633  C   MET A 457      13.454   6.866  34.580  1.00  2.43           C
ATOM    634  O   MET A 457      14.312   7.094  35.376  1.00  2.00           O
ATOM    635  N   GLU A 458      12.217   6.546  34.941  1.00  3.37           N
ATOM    636  CA  GLU A 458      11.796   6.489  36.329  1.00  4.85           C
ATOM    637  CB  GLU A 458      10.250   6.508  36.461  1.00  6.22           C
ATOM    638  CG  GLU A 458       9.743   6.297  37.876  1.00  9.88           C
ATOM    639  CD  GLU A 458       8.217   6.296  38.008  1.00 16.41           C
ATOM    640  OE1 GLU A 458       7.728   6.142  39.145  1.00 16.60           O
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ATOM    641  OE2 GLU A 458       7.494   6.470  36.992  1.00 21.88           O
ATOM    642  C   GLU A 458      12.397   5.295  37.024  1.00  3.62           C
ATOM    643  O   GLU A 458      12.707   5.380  38.188  1.00  2.58           O
ATOM    644  N   SER A 459      12.607   4.189  36.300  1.00  3.61           N
ATOM    645  CA  SER A 459      13.252   3.018  36.912  1.00  2.73           C
ATOM    646  CB  SER A 459      13.078   1.796  36.043  1.00  2.08           C
ATOM    647  OG  SER A 459      13.733   0.633  36.548  1.00  2.00           O
ATOM    648  C   SER A 459      14.736   3.330  37.168  1.00  3.70           C
ATOM    649  O   SER A 459      15.297   2.986  38.201  1.00  2.47           O
ATOM    650  N   MET A 460      15.368   4.020  36.230  1.00  4.07           N
ATOM    651  CA  MET A 460      16.754   4.383  36.433  1.00  4.93           C
ATOM    652  CB  MET A 460      17.361   5.054  35.178  1.00  4.86           C
ATOM    653  CG  MET A 460      17.501   4.164  33.993  1.00  8.07           C
ATOM    654  SD  MET A 460      18.246   4.959  32.523  1.00 13.32           S
ATOM    655  CE  MET A 460      18.698   3.528  31.591  1.00 10.36           C
ATOM    656  C   MET A 460      16.909   5.320  37.641  1.00  5.63           C
ATOM    657  O   MET A 460      17.854   5.152  38.423  1.00  5.63           O
ATOM    658  N   LEU A 461      16.023   6.318  37.767  1.00  5.49           N
ATOM    659  CA  LEU A 461      16.142   7.295  38.821  1.00  6.56           C
ATOM    660  CB  LEU A 461      15.134   8.436  38.604  1.00  6.42           C
ATOM    661  CG  LEU A 461      15.377   9.443  37.446  1.00  6.02           C
ATOM    662  CD1 LEU A 461      14.169  10.331  37.283  1.00  2.12           C
ATOM    663  CD2 LEU A 461      16.678  10.249  37.573  1.00  2.00           C
ATOM    664  C   LEU A 461      15.932   6.630  40.218  1.00  8.27           C
ATOM    665  O   LEU A 461      16.665   6.892  41.159  1.00  7.16           O
ATOM    666  N   LYS A 462      14.903   5.799  40.351  1.00 10.76           N
ATOM    667  CA  LYS A 462      14.653   5.106  41.623  1.00 13.62           C
ATOM    668  CB  LYS A 462      13.464   4.156  41.578  1.00 13.89           C
ATOM    669  CG  LYS A 462      12.086   4.865  41.307  1.00 17.14           C
ATOM    670  CD  LYS A 462      10.931   3.852  41.398  1.00 20.36           C
ATOM    671  CE  LYS A 462       9.546   4.493  41.278  1.00 19.96           C
ATOM    672  NZ  LYS A 462       8.469   3.509  41.729  1.00 17.73           N
ATOM    673  C   LYS A 462      15.886   4.330  41.985  1.00 13.79           C
ATOM    674  O   LYS A 462      16.346   4.384  43.137  1.00 15.92           O
ATOM    675  N   SER A 463      16.491   3.733  40.987  1.00 12.72           N
ATOM    676  CA  SER A 463      17.684   2.995  41.195  1.00 13.57           C
ATOM    677  CB  SER A 463      18.055   2.288  39.926  1.00 14.00           C
ATOM    678  OG  SER A 463      19.089   1.391  40.192  1.00 13.63           O
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ATOM    679  C   SER A 463      18.862   3.837  41.628  1.00 14.52           C
ATOM    680  O   SER A 463      19.609   3.479  42.533  1.00 15.99           O
ATOM    681  N   GLU A 464      19.070   4.958  40.971  1.00 14.97           N
ATOM    682  CA  GLU A 464      20.196   5.767  41.321  1.00 14.47           C
ATOM    683  CB  GLU A 464      20.352   6.912  40.359  1.00 13.37           C
ATOM    684  CG  GLU A 464      21.027   6.509  39.072  1.00 15.00           C
ATOM    685  CD  GLU A 464      22.427   5.984  39.244  1.00 13.58           C
ATOM    686  OE1 GLU A 464      22.561   5.003  39.965  1.00 17.87           O
ATOM    687  OE2 GLU A 464      23.388   6.526  38.654  1.00 12.54           O
ATOM    688  C   GLU A 464      20.064   6.271  42.729  1.00 15.03           C
ATOM    689  O   GLU A 464      21.057   6.362  43.440  1.00 13.80           O
ATOM    690  N   GLU A 465      18.835   6.619  43.107  1.00 16.34           N
ATOM    691  CA  GLU A 465      18.551   7.176  44.428  1.00 18.04           C
ATOM    692  CB  GLU A 465      17.056   7.574  44.544  1.00 17.67           C
ATOM    693  CG  GLU A 465      16.680   8.192  45.889  1.00 19.26           C
ATOM    694  CD  GLU A 465      15.185   8.431  46.085  1.00 21.39           C
ATOM    695  OE1 GLU A 465      14.733   8.538  47.260  1.00 24.00           O
ATOM    696  OE2 GLU A 465      14.460   8.543  45.086  1.00 20.75           O
ATOM    697  C   GLU A 465      18.981   6.218  45.554  1.00 18.80           C
ATOM    698  O   GLU A 465      19.486   6.627  46.552  1.00 18.58           O
ATOM    699  N   GLU A 466      18.818   4.922  45.356  1.00 21.36           N
ATOM    700  CA  GLU A 466      19.154   3.978  46.399  1.00 23.94           C
ATOM    701  CB  GLU A 466      18.257   2.740  46.301  1.00 24.78           C
ATOM    702  CG  GLU A 466      18.800   1.694  45.376  1.00 31.30           C
ATOM    703  CD  GLU A 466      18.024   0.404  45.467  1.00 37.63           C
ATOM    704  OE1 GLU A 466      17.805  -0.006  46.641  1.00 39.08           O
ATOM    705  OE2 GLU A 466      17.638  -0.157  44.382  1.00 36.89           O
ATOM    706  C   GLU A 466      20.600   3.578  46.356  1.00 23.81           C
ATOM    707  O   GLU A 466      21.106   2.912  47.247  1.00 23.07           O
ATOM    708  N   ARG A 467      21.257   3.973  45.272  1.00 25.21           N
ATOM    709  CA  ARG A 467      22.666   3.659  45.051  1.00 24.44           C
ATOM    710  CB  ARG A 467      22.925   3.465  43.576  1.00 23.48           C
ATOM    711  CG  ARG A 467      24.352   3.283  43.224  1.00 21.88           C
ATOM    712  CD  ARG A 467      24.659   3.512  41.707  1.00 20.93           C
ATOM    713  NE  ARG A 467      26.015   4.022  41.616  1.00 18.63           N
ATOM    714  CZ  ARG A 467      26.367   5.089  40.982  1.00 15.74           C
ATOM    715  NH1 ARG A 467      25.481   5.760  40.281  1.00 12.88           N
ATOM    716  NH2 ARG A 467      27.641   5.467  41.027  1.00 18.41           N
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ATOM    717  C   ARG A 467      23.560   4.765  45.573  1.00 24.26           C
ATOM    718  O   ARG A 467      24.669   4.516  45.988  1.00 25.68           O
ATOM    719  N   LEU A 468      23.067   5.979  45.572  1.00 23.45           N
ATOM    720  CA  LEU A 468      23.871   7.109  45.983  1.00 23.85           C
ATOM    721  CB  LEU A 468      24.092   8.052  44.801  1.00 23.40           C
ATOM    722  CG  LEU A 468      24.921   7.685  43.581  1.00 23.39           C
ATOM    723  CD1 LEU A 468      24.393   8.459  42.390  1.00 19.92           C
ATOM    724  CD2 LEU A 468      26.380   8.047  43.836  1.00 25.54           C
ATOM    725  C   LEU A 468      23.174   7.919  47.087  1.00 24.22           C
ATOM    726  O   LEU A 468      23.753   8.862  47.608  1.00 23.40           O
ATOM    727  N   SER A 469      21.940   7.549  47.427  1.00 24.43           N
ATOM    728  CA  SER A 469      21.160   8.357  48.310  1.00 25.52           C
ATOM    729  CB  SER A 469      21.893   8.580  49.621  1.00 26.28           C
ATOM    730  OG  SER A 469      22.034   7.352  50.339  1.00 24.93           O
ATOM    731  C   SER A 469      21.022   9.644  47.500  1.00 26.91           C
ATOM    732  O   SER A 469      21.227   9.627  46.285  1.00 28.46           O
ATOM    733  N   ILE A 470      20.666  10.774  48.091  1.00 26.91           N
ATOM    734  CA  ILE A 470      20.567  11.941  47.218  1.00 25.86           C
ATOM    735  CB  ILE A 470      21.907  12.106  46.458  1.00 25.79           C
ATOM    736  CG1 ILE A 470      22.706  13.245  47.112  1.00 26.46           C
ATOM    737  CD1 ILE A 470      24.137  13.426  46.636  1.00 28.15           C
ATOM    738  CG2 ILE A 470      21.697  12.313  44.944  1.00 25.97           C
ATOM    739  C   ILE A 470      19.406  11.815  46.260  1.00 25.84           C
ATOM    740  O   ILE A 470      19.196  10.760  45.661  1.00 23.67           O
ATOM    741  N   GLN A 471      18.600  12.878  46.174  1.00 26.30           N
ATOM    742  CA  GLN A 471      17.516  12.894  45.210  1.00 27.70           C
ATOM    743  CB  GLN A 471      16.221  13.383  45.835  1.00 28.63           C
ATOM    744  CG  GLN A 471      15.514  12.376  46.723  1.00 32.75           C
ATOM    745  CD  GLN A 471      16.285  12.086  48.043  1.00 38.95           C
ATOM    746  OE1 GLN A 471      16.536  13.000  48.845  1.00 36.46           O
ATOM    747  NE2 GLN A 471      16.656  10.801  48.257  1.00 41.47           N
ATOM    748  C   GLN A 471      18.005  13.851  44.141  1.00 27.03           C
ATOM    749  O   GLN A 471      19.174  13.799  43.776  1.00 28.39           O
ATOM    750  N   ASN A 472      17.163  14.703  43.585  1.00 25.58           N
ATOM    751  CA  ASN A 472      17.755  15.736  42.680  1.00 25.14           C
ATOM    752  CB  ASN A 472      18.985  16.425  43.345  1.00 24.93           C
ATOM    753  CG  ASN A 472      19.348  17.803  42.708  1.00 28.30           C
ATOM    754  OD1 ASN A 472      19.877  18.682  43.390  1.00 23.38           O
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ATOM    755  ND2 ASN A 472      19.073  17.974  41.391  1.00 29.82           N
ATOM    756  C   ASN A 472      18.118  15.198  41.256  1.00 22.63           C
ATOM    757  O   ASN A 472      17.204  14.902  40.446  1.00 21.83           O
ATOM    758  N   PHE A 473      19.419  15.043  40.990  1.00 19.00           N
ATOM    759  CA  PHE A 473      19.885  14.539  39.654  1.00 17.56           C
ATOM    760  CB  PHE A 473      19.095  13.278  39.175  1.00 15.51           C
ATOM    761  CG  PHE A 473      19.295  12.095  40.041  1.00 14.08           C
ATOM    762  CD1 PHE A 473      18.379  11.788  41.031  1.00 14.53           C
ATOM    763  CE1 PHE A 473      18.603  10.715  41.900  1.00 11.36           C
ATOM    764  CZ  PHE A 473      19.726   9.961  41.785  1.00  8.01           C
ATOM    765  CE2 PHE A 473      20.648  10.257  40.810  1.00 10.92           C
ATOM    766  CD2 PHE A 473      20.444  11.329  39.954  1.00 13.01           C
ATOM    767  C   PHE A 473      19.944  15.623  38.527  1.00 15.68           C
ATOM    768  O   PHE A 473      20.018  15.264  37.360  1.00 15.69           O
ATOM    769  N   SER A 474      19.930  16.910  38.897  1.00 13.72           N
ATOM    770  CA  SER A 474      19.840  18.016  37.936  1.00 13.11           C
ATOM    771  CB  SER A 474      20.136  19.379  38.604  1.00 14.23           C
ATOM    772  OG  SER A 474      19.705  20.550  37.894  1.00  6.19           O
ATOM    773  C   SER A 474      20.702  17.877  36.691  1.00 13.44           C
ATOM    774  O   SER A 474      20.221  18.062  35.597  1.00 13.49           O
ATOM    775  N   LYS A 475      21.978  17.578  36.867  1.00 13.37           N
ATOM    776  CA  LYS A 475      22.878  17.435  35.754  1.00 12.47           C
ATOM    777  CB  LYS A 475      24.286  17.089  36.185  1.00 12.77           C
ATOM    778  CG  LYS A 475      25.288  17.204  35.033  1.00 13.73           C
ATOM    779  CD  LYS A 475      26.724  17.423  35.480  1.00 16.66           C
ATOM    780  CE  LYS A 475      27.742  17.332  34.315  1.00 24.37           C
ATOM    781  NZ  LYS A 475      27.400  18.006  32.937  1.00 23.53           N
ATOM    782  C   LYS A 475      22.467  16.436  34.747  1.00 12.94           C
ATOM    783  O   LYS A 475      22.438  16.736  33.530  1.00 14.20           O
ATOM    784  N   LEU A 476      22.188  15.223  35.203  1.00 12.84           N
ATOM    785  CA  LEU A 476      21.832  14.124  34.294  1.00 11.68           C
ATOM    786  CB  LEU A 476      21.567  12.879  35.056  1.00 11.55           C
ATOM    787  CG  LEU A 476      21.072  11.659  34.255  1.00 14.10           C
ATOM    788  CD1 LEU A 476      21.999  11.262  33.212  1.00 12.17           C
ATOM    789  CD2 LEU A 476      20.899  10.436  35.250  1.00 14.83           C
ATOM    790  C   LEU A 476      20.597  14.474  33.514  1.00 11.27           C
ATOM    791  O   LEU A 476      20.608  14.449  32.289  1.00 11.58           O
ATOM    792  N   LEU A 477      19.554  14.876  34.234  1.00  9.67           N
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ATOM    793  CA  LEU A 477      18.271  15.210  33.633  1.00  7.27           C
ATOM    794  CB  LEU A 477      17.211  15.256  34.724  1.00  6.59           C
ATOM    795  CG  LEU A 477      17.000  13.934  35.430  1.00  6.22           C
ATOM    796  CD1 LEU A 477      15.877  14.102  36.533  1.00  2.69           C
ATOM    797  CD2 LEU A 477      16.667  12.908  34.367  1.00  2.00           C
ATOM    798  C   LEU A 477      18.236  16.520  32.794  1.00  6.03           C
ATOM    799  O   LEU A 477      17.234  16.807  32.164  1.00  5.74           O
ATOM    800  N   ASN A 478      19.283  17.310  32.784  1.00  4.35           N
ATOM    801  CA  ASN A 478      19.264  18.470  31.877  1.00  6.17           C
ATOM    802  CB  ASN A 478      19.716  19.783  32.539  1.00  5.15           C
ATOM    803  CG  ASN A 478      18.612  20.397  33.419  1.00  5.45           C
ATOM    804  OD1 ASN A 478      17.615  20.849  32.868  1.00  6.20           O
ATOM    805  ND2 ASN A 478      18.764  20.374  34.773  1.00  2.00           N
ATOM    806  C   ASN A 478      20.057  18.257  30.562  1.00  6.46           C
ATOM    807  O   ASN A 478      20.037  19.127  29.680  1.00  6.14           O
ATOM    808  N   ASP A 479      20.712  17.098  30.461  1.00  5.99           N
ATOM    809  CA  ASP A 479      21.572  16.766  29.360  1.00  7.55           C
ATOM    810  CB  ASP A 479      22.520  15.643  29.755  1.00  7.69           C
ATOM    811  CG  ASP A 479      23.519  15.344  28.706  1.00 12.13           C
ATOM    812  OD1 ASP A 479      23.206  15.086  27.511  1.00 18.57           O
ATOM    813  OD2 ASP A 479      24.708  15.317  28.984  1.00 21.87           O
ATOM    814  C   ASP A 479      20.791  16.305  28.146  1.00  7.54           C
ATOM    815  O   ASP A 479      20.205  15.236  28.165  1.00  8.94           O
ATOM    816  N   ASN A 480      20.893  17.062  27.063  1.00  6.80           N
ATOM    817  CA  ASN A 480      20.198  16.762  25.841  1.00  5.52           C
ATOM    818  CB  ASN A 480      20.510  17.835  24.799  1.00  4.25           C
ATOM    819  CG  ASN A 480      19.772  17.630  23.540  1.00  5.64           C
ATOM    820  OD1 ASN A 480      20.369  17.413  22.488  1.00 13.62           O
ATOM    821  ND2 ASN A 480      18.463  17.638  23.620  1.00  5.94           N
ATOM    822  C   ASN A 480      20.522  15.352  25.332  1.00  4.85           C
ATOM    823  O   ASN A 480      19.612  14.554  25.048  1.00  2.00           O
ATOM    824  N   ILE A 481      21.812  15.051  25.262  1.00  5.91           N
ATOM    825  CA  ILE A 481      22.281  13.726  24.790  1.00  6.95           C
ATOM    826  CB  ILE A 481      23.805  13.604  24.829  1.00  7.62           C
ATOM    827  CG1 ILE A 481      24.480  14.691  23.972  1.00  8.74           C
ATOM    828  CD1 ILE A 481      24.208  14.429  22.466  1.00 17.85           C
ATOM    829  CG2 ILE A 481      24.205  12.265  24.282  1.00  7.84           C
ATOM    830  C   ILE A 481      21.713  12.560  25.551  1.00  6.93           C
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ATOM    831  O   ILE A 481      21.364  11.555  24.932  1.00  8.37           O
ATOM    832  N   PHE A 482      21.656  12.660  26.879  1.00  5.61           N
ATOM    833  CA  PHE A 482      21.076  11.595  27.710  1.00  4.96           C
ATOM    834  CB  PHE A 482      21.064  11.967  29.220  1.00  3.95           C
ATOM    835  CG  PHE A 482      20.218  11.064  30.044  1.00  2.00           C
ATOM    836  CD1 PHE A 482      20.616   9.760  30.273  1.00  2.30           C
ATOM    837  CE1 PHE A 482      19.779   8.872  31.037  1.00  4.02           C
ATOM    838  CZ  PHE A 482      18.537   9.353  31.571  1.00  6.39           C
ATOM    839  CE2 PHE A 482      18.140  10.701  31.307  1.00  3.09           C
ATOM    840  CD2 PHE A 482      18.986  11.517  30.569  1.00  2.00           C
ATOM    841  C   PHE A 482      19.631  11.205  27.303  1.00  4.81           C
ATOM    842  O   PHE A 482      19.379  10.044  27.144  1.00  4.61           O
ATOM    843  N   HIS A 483      18.721  12.184  27.192  1.00  3.46           N
ATOM    844  CA  HIS A 483      17.323  11.995  26.803  1.00  4.48           C
ATOM    845  CB  HIS A 483      16.500  13.264  27.001  1.00  3.03           C
ATOM    846  CG  HIS A 483      16.343  13.637  28.434  1.00  6.88           C
ATOM    847  ND1 HIS A 483      15.533  12.932  29.305  1.00  5.16           N
ATOM    848  CE1 HIS A 483      15.629  13.475  30.504  1.00  6.16           C
ATOM    849  NE2 HIS A 483      16.479  14.482  30.451  1.00  4.45           N
ATOM    850  CD2 HIS A 483      16.956  14.590  29.173  1.00  5.78           C
ATOM    851  C   HIS A 483      17.210  11.610  25.339  1.00  4.68           C
ATOM    852  O   HIS A 483      16.287  10.899  24.919  1.00  4.81           O
ATOM    853  N   MET A 484      18.163  12.066  24.564  1.00  4.57           N
ATOM    854  CA  MET A 484      18.143  11.733  23.163  1.00  5.49           C
ATOM    855  CB  MET A 484      19.135  12.555  22.454  1.00  5.43           C
ATOM    856  CG  MET A 484      18.627  13.127  21.223  1.00 13.21           C
ATOM    857  SD  MET A 484      17.108  14.107  21.275  1.00 15.95           S
ATOM    858  CE  MET A 484      17.888  15.586  21.607  1.00 23.47           C
ATOM    859  C   MET A 484      18.512  10.264  23.026  1.00  4.72           C
ATOM    860  O   MET A 484      17.927   9.590  22.188  1.00  4.49           O
ATOM    861  N   SER A 485      19.399   9.758  23.892  1.00  2.84           N
ATOM    862  CA  SER A 485      19.863   8.378  23.799  1.00  3.18           C
ATOM    863  CB  SER A 485      21.196   8.206  24.505  1.00  4.17           C
ATOM    864  OG  SER A 485      22.253   8.922  23.891  1.00  5.43           O
ATOM    865  C   SER A 485      18.866   7.382  24.382  1.00  2.76           C
ATOM    866  O   SER A 485      18.580   6.323  23.797  1.00  3.40           O
ATOM    867  N   LEU A 486      18.291   7.753  25.499  1.00  2.70           N
ATOM    868  CA  LEU A 486      17.294   6.932  26.173  1.00  2.83           C
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ATOM    869  CB  LEU A 486      16.795   7.645  27.456  1.00  2.69           C
ATOM    870  CG  LEU A 486      16.678   6.926  28.798  1.00  5.49           C
ATOM    871 CD1 LEU A 486      15.484   7.415  29.632  1.00  2.00           C
ATOM    872 CD2 LEU A 486      16.643   5.426  28.695  1.00  7.92           C
ATOM    873  C   LEU A 486      16.135   6.698  25.188  1.00  2.25           C
ATOM    874  O   LEU A 486      15.750   5.566  24.970  1.00  2.40           O
ATOM    875  N   LEU A 487      15.645   7.774  24.562  1.00  2.00           N
ATOM    876  CA  LEU A 487      14.480   7.731  23.690  1.00  3.45           C
ATOM    877  CB  LEU A 487      14.104   9.150  23.196  1.00  4.14           C
ATOM    878  CG  LEU A 487      12.637   9.614  23.068  1.00  5.86           C
ATOM    879 CD1 LEU A 487      12.505  10.719  21.953  1.00  4.99           C
ATOM    880 CD2 LEU A 487      11.658   8.512  22.759  1.00  7.08           C
ATOM    881  C   LEU A 487      14.718   6.785  22.477  1.00  3.80           C
ATOM    882  O   LEU A 487      13.887   5.903  22.194  1.00  2.00           O
ATOM    883  N   ALA A 488      15.873   6.983  21.838  1.00  3.28           N
ATOM    884  CA  ALA A 488      16.299   6.192  20.698  1.00  4.99           C
ATOM    885  CB  ALA A 488      17.695   6.594  20.270  1.00  5.66           C
ATOM    886  C   ALA A 488      16.341   4.758  21.092  1.00  5.49           C
ATOM    887  O   ALA A 488      15.806   3.885  20.441  1.00  6.07           O
ATOM    888  N   CYS A 489      16.993   4.496  22.198  1.00  6.10           N
ATOM    889  CA  CYS A 489      17.122   3.122  22.588  1.00  5.29           C
ATOM    890  CB  CYS A 489      17.998   3.023  23.837  1.00  4.37           C
ATOM    891  SG  CYS A 489      18.230   1.310  24.279  1.00  5.78           S
ATOM    892  C   CYS A 489      15.738   2.513  22.729  1.00  5.44           C
ATOM    893  O   CYS A 489      15.444   1.438  22.163  1.00  4.75           O
ATOM    894  N   ALA A 490      14.888   3.233  23.462  1.00  5.61           N
ATOM    895  CA  ALA A 490      13.503   2.829  23.673  1.00  5.43           C
ATOM    896  CB  ALA A 490      12.815   3.780  24.604  1.00  6.08           C
ATOM    897  C   ALA A 490      12.700   2.669  22.406  1.00  4.62           C
ATOM    898  O   ALA A 490      11.860   1.779  22.335  1.00  6.60           O
ATOM    899  N   LEU A 491      12.957   3.472  21.395  1.00  3.23           N
ATOM    900  CA  LEU A 491      12.237   3.330  20.140  1.00  2.52           C
ATOM    901  CB  LEU A 491      12.343   4.622  19.349  1.00  2.72           C
ATOM    902  CG  LEU A 491      11.536   5.885  19.661  1.00  2.48           C
ATOM    903 CD1 LEU A 491      12.083   7.153  18.984  1.00  2.00           C
ATOM    904 CD2 LEU A 491      10.047   5.660  19.324  1.00  2.00           C
ATOM    905  C   LEU A 491      12.851   2.178  19.332  1.00  3.77           C
ATOM    906  O   LEU A 491      12.243   1.614  18.485  1.00  3.11           O
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ATOM    907  N   GLU A 492      14.109   1.865  19.555  1.00  5.20           N
ATOM    908  CA  GLU A 492      14.694   0.850  18.745  1.00  7.70           C
ATOM    909  CB  GLU A 492      16.201   0.864  18.909  1.00  7.57           C
ATOM    910  CG  GLU A 492      16.964  -0.236  18.193  1.00 10.36           C
ATOM    911  CD  GLU A 492      16.581  -0.371  16.735  1.00 12.45           C
ATOM    912  OE1 GLU A 492      16.431   0.631  16.081  1.00 17.37           O
ATOM    913  OE2 GLU A 492      16.433  -1.468  16.213  1.00 14.99           O
ATOM    914  C   GLU A 492      14.102  -0.480  19.162  1.00  9.34           C
ATOM    915  O   GLU A 492      13.919  -1.384  18.346  1.00  9.42           O
ATOM    916  N   VAL A 493      13.806  -0.597  20.445  1.00 10.25           N
ATOM    917  CA  VAL A 493      13.230  -1.804  20.970  1.00 10.00           C
ATOM    918  CB  VAL A 493      13.208  -1.735  22.536  1.00 11.55           C
ATOM    919  CG1 VAL A 493      12.173  -2.764  23.129  1.00  8.23           C
ATOM    920  CG2 VAL A 493      14.608  -1.955  23.072  1.00  7.40           C
ATOM    921  C   VAL A 493      11.802  -1.988  20.466  1.00 10.30           C
ATOM    922  O   VAL A 493      11.449  -3.037  20.047  1.00 10.69           O
ATOM    923  N   VAL A 494      11.016  -0.926  20.434  1.00 10.67           N
ATOM    924  CA  VAL A 494       9.637  -1.000  20.006  1.00 10.15           C
ATOM    925  CB  VAL A 494       8.838   0.337  20.293  1.00  9.64           C
ATOM    926  CG1 VAL A 494       7.530   0.329  19.610  1.00  6.54           C
ATOM    927  CG2 VAL A 494       8.558   0.545  21.852  1.00  6.43           C
ATOM    928  C   VAL A 494       9.550  -1.362  18.563  1.00 12.13           C
ATOM    929  O   VAL A 494       8.754  -2.219  18.178  1.00 12.62           O
ATOM    930  N   MET A 495      10.363  -0.722  17.742  1.00 13.37           N
ATOM    931  CA  MET A 495      10.344  -1.038  16.324  1.00 15.28           C
ATOM    932  CB  MET A 495      11.097   0.035  15.531  1.00 14.65           C
ATOM    933  CG  MET A 495      10.405   1.316  15.544  1.00 13.27           C
ATOM    934  SD  MET A 495      11.314   2.329  14.534  1.00 18.39           S
ATOM    935  CE  MET A 495      10.911   1.751  12.891  1.00 23.19           C
ATOM    936  C   MET A 495      10.876  -2.438  15.991  1.00 16.42           C
ATOM    937  O   MET A 495      10.586  -2.968  14.935  1.00 15.60           O
ATOM    938  N   ALA A 496      11.688  -2.993  16.884  1.00 18.74           N
ATOM    939  CA  ALA A 496      12.290  -4.310  16.687  1.00 21.16           C
ATOM    940  CB  ALA A 496      13.319  -4.623  17.755  1.00 20.54           C
ATOM    941  C   ALA A 496      11.219  -5.344  16.778  1.00 23.00           C
ATOM    942  O   ALA A 496      11.094  -6.267  15.922  1.00 22.03           O
ATOM    943  N   THR A 497      10.445  -5.221  17.836  1.00 24.64           N
ATOM    944  CA  THR A 497       9.436  -6.220  18.009  1.00 27.98           C
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ATOM    945  CB  THR A 497       8.657  -5.942  19.223  1.00 27.33           C
ATOM    946  OG1 THR A 497       7.876  -4.776  18.968  1.00 29.40           O
ATOM    947  CG2 THR A 497       9.609  -5.593  20.366  1.00 25.14           C
ATOM    948  C   THR A 497       8.512  -6.334  16.784  1.00 30.44           C
ATOM    949  O   THR A 497       8.060  -7.443  16.457  1.00 30.05           O
ATOM    950  N   TYR A 498       8.256  -5.210  16.104  1.00 33.44           N
ATOM    951  CA  TYR A 498       7.368  -5.204  14.927  1.00 36.84           C
ATOM    952  CB  TYR A 498       6.363  -4.042  14.984  1.00 36.22           C
ATOM    953  CG  TYR A 498       5.695  -3.904  16.329  1.00 37.40           C
ATOM    954  CD1 TYR A 498       4.755  -4.822  16.756  1.00 39.74           C
ATOM    955  CE1 TYR A 498       4.162  -4.693  18.018  1.00 41.01           C
ATOM    956  CZ  TYR A 498       4.520  -3.631  18.828  1.00 38.06           C
ATOM    957  OH  TYR A 498       3.974  -3.454  20.077  1.00 38.69           O
ATOM    958  CE2 TYR A 498       5.443  -2.731  18.404  1.00 35.90           C
ATOM    959  CD2 TYR A 498       6.019  -2.865  17.183  1.00 35.68           C
ATOM    960  C   TYR A 498       8.074  -5.242  13.556  1.00 39.17           C
ATOM    961  O   TYR A 498       7.561  -4.693  12.563  1.00 40.64           O
ATOM    962  N   SER A 499       9.233  -5.887  13.478  1.00 41.51           N
ATOM    963  CA  SER A 499       9.962  -5.935  12.205  1.00 43.56           C
ATOM    964  CB  SER A 499      11.290  -6.704  12.338  1.00 43.58           C
ATOM    965  OG  SER A 499      12.305  -5.924  12.951  1.00 41.96           O
ATOM    966  C   SER A 499       9.098  -6.527  11.084  1.00 45.17           C
ATOM    967  O   SER A 499       9.103  -5.993   9.973  1.00 45.09           O
ATOM    968  N   ARG A 500       8.382  -7.631  11.378  1.00 46.76           N
ATOM    969  CA  ARG A 500       7.476  -8.292  10.409  1.00 48.01           C
ATOM    970  CB  ARG A 500       7.233  -9.738  10.797  1.00 47.71           C
ATOM    971  CG  ARG A 500       6.773 -10.619   9.631  1.00 49.22           C
ATOM    972  CD  ARG A 500       5.473 -11.420   9.915  1.00 50.50           C
ATOM    973  NE  ARG A 500       4.297 -10.547  10.020  1.00 52.41           N
ATOM    974  CZ  ARG A 500       3.024 -10.961  10.043  1.00 52.33           C
ATOM    975  NH1 ARG A 500       2.726 -12.270   9.976  1.00 49.40           N
ATOM    976  NH2 ARG A 500       2.045 -10.052  10.132  1.00 49.92           N
ATOM    977  C   ARG A 500       6.124  -7.563  10.321  1.00 48.87           C
ATOM    978  O   ARG A 500       5.050  -8.171  10.489  1.00 48.55           O
ATOM    979  N   SER A 501       6.211  -6.248  10.092  1.00 49.79           N
ATOM    980  CA  SER A 501       5.058  -5.356   9.992  1.00 50.64           C
ATOM    981  CB  SER A 501       5.166  -4.236  11.026  1.00 50.82           C
ATOM    982  OG  SER A 501       4.077  -3.328  10.893  1.00 51.88           O
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ATOM    983  C   SER A 501       4.924  -4.738   8.587  1.00 50.90           C
ATOM    984  O   SER A 501       3.844  -4.752   7.983  1.00 50.85           O
ATOM    985  N   SER A 508       9.297   1.112  -0.283  1.00 57.14           N
ATOM    986  CA  SER A 508      10.177   0.166   0.420  1.00 56.24           C
ATOM    987  CB  SER A 508      10.072  -1.239  -0.219  1.00 56.13           C
ATOM    988  OG  SER A 508       8.726  -1.704  -0.216  1.00 54.22           O
ATOM    989  C   SER A 508      11.636   0.689   0.478  1.00 55.73           C
ATOM    990  O   SER A 508      12.609  -0.084   0.559  1.00 56.00           O
ATOM    991  N   GLY A 509      11.773   2.013   0.436  1.00 54.44           N
ATOM    992  CA  GLY A 509      13.075   2.644   0.499  1.00 52.95           C
ATOM    993  C   GLY A 509      13.712   2.435   1.851  1.00 51.71           C
ATOM    994  O   GLY A 509      14.026   3.403   2.552  1.00 51.34           O
ATOM    995  N   THR A 510      13.924   1.160   2.179  1.00 50.64           N
ATOM    996  CA  THR A 510      14.498   0.702   3.455  1.00 49.39           C
ATOM    997  CB  THR A 510      16.036   0.527   3.429  1.00 50.13           C
ATOM    998  OG1 THR A 510      16.487   0.219   4.774  1.00 49.53           O
ATOM    999  CG2 THR A 510      16.783   1.834   3.003  1.00 49.41           C
ATOM   1000  C   THR A 510      14.164   1.482   4.674  1.00 48.11           C
ATOM   1001  O   THR A 510      14.292   2.708   4.691  1.00 48.23           O
ATOM   1002  N   ASP A 511      13.774   0.760   5.719  1.00 46.68           N
ATOM   1003  CA  ASP A 511      13.456   1.400   6.998  1.00 44.62           C
ATOM   1004  CB  ASP A 511      12.053   1.024   7.442  1.00 45.05           C
ATOM   1005  CG  ASP A 511      11.752   1.485   8.823  1.00 44.34           C
ATOM   1006  OD1 ASP A 511      11.716   2.709   9.062  1.00 47.00           O
ATOM   1007  OD2 ASP A 511      11.556   0.693   9.743  1.00 43.18           O
ATOM   1008  C   ASP A 511      14.454   1.018   8.093  1.00 42.93           C
ATOM   1009  O   ASP A 511      15.641   0.716   7.827  1.00 42.65           O
ATOM   1010  N   LEU A 512      13.953   1.009   9.322  1.00 40.19           N
ATOM   1011  CA  LEU A 512      14.792   0.764  10.492  1.00 37.10           C
ATOM   1012  CB  LEU A 512      13.935   0.548  11.720  1.00 36.88           C
ATOM   1013  CG  LEU A 512      14.573   0.486  13.093  1.00 38.65           C
ATOM   1014  CD1 LEU A 512      15.068  -0.968  13.429  1.00 39.66           C
ATOM   1015  CD2 LEU A 512      15.676   1.573  13.278  1.00 39.27           C
ATOM   1016  C   LEU A 512      15.743  -0.390  10.273  1.00 34.87           C
ATOM   1017  O   LEU A 512      15.760  -1.031   9.220  1.00 34.35           O
ATOM   1018  N   SER A 513      16.542  -0.607  11.299  1.00 32.30           N
ATOM   1019  CA  SER A 513      17.599  -1.586  11.342  1.00 29.77           C
ATOM   1020  CB  SER A 513      18.113  -1.943   9.931  1.00 30.70           C
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ATOM   1021  OG  SER A 513      17.245  -2.859   9.250  1.00 30.48           O
ATOM   1022  C   SER A 513      18.597  -0.743  12.154  1.00 26.48           C
ATOM   1023  O   SER A 513      19.360   0.031  11.624  1.00 25.26           O
ATOM   1024  N   PHE A 514      18.537  -0.922  13.460  1.00 23.05           N
ATOM   1025  CA  PHE A 514      19.332  -0.177  14.402  1.00 19.60           C
ATOM   1026  CB  PHE A 514      20.495  -0.914  14.932  1.00 17.88           C
ATOM   1027  CG  PHE A 514      21.410  -0.038  15.659  1.00 13.56           C
ATOM   1028  CD1 PHE A 514      22.774  -0.135  15.466  1.00  7.78           C
ATOM   1029  CE1 PHE A 514      23.601   0.675  16.127  1.00  7.61           C
ATOM   1030  CZ  PHE A 514      23.077   1.632  17.011  1.00 10.61           C
ATOM   1031  CE2 PHE A 514      21.715   1.743  17.219  1.00  5.65           C
ATOM   1032  CD2 PHE A 514      20.893   0.919  16.539  1.00  7.37           C
ATOM   1033  C   PHE A 514      19.831   1.160  13.883  1.00 19.98           C
ATOM   1034  O   PHE A 514      19.175   2.200  14.198  1.00 21.97           O
ATOM   1035  N   PRO A 515      20.917   1.189  13.071  1.00 16.87           N
ATOM   1036  CA  PRO A 515      21.498   2.461  12.678  1.00 13.02           C
ATOM   1037  CB  PRO A 515      22.506   2.056  11.613  1.00 13.72           C
ATOM   1038  CG  PRO A 515      22.040   0.796  11.161  1.00 13.79           C
ATOM   1039  CD  PRO A 515      21.587   0.062  12.404  1.00 16.21           C
ATOM   1040  C   PRO A 515      20.449   3.495  12.185  1.00 11.10           C
ATOM   1041  O   PRO A 515      20.673   4.693  12.490  1.00 11.58           O
ATOM   1042  N   TRP A 516      19.356   3.097  11.514  1.00  8.08           N
ATOM   1043  CA  TRP A 516      18.374   4.084  10.997  1.00  6.57           C
ATOM   1044  CB  TRP A 516      17.119   3.393  10.446  1.00  6.20           C
ATOM   1045  CG  TRP A 516      16.106   4.310   9.797  1.00  6.53           C
ATOM   1046  CD1 TRP A 516      16.196   4.932   8.538  1.00  6.10           C
ATOM   1047  NE1 TRP A 516      15.058   5.663   8.286  1.00  2.00           N
ATOM   1048  CE2 TRP A 516      14.229   5.565   9.354  1.00  2.00           C
ATOM   1049  CD2 TRP A 516      14.860   4.732  10.333  1.00  3.32           C
ATOM   1050  CE3 TRP A 516      14.213   4.528  11.555  1.00  2.00           C
ATOM   1051  CZ3 TRP A 516      12.976   5.088  11.741  1.00  2.00           C
ATOM   1052  CH2 TRP A 516      12.376   5.861  10.761  1.00  2.00           C
ATOM   1053  CZ2 TRP A 516      13.015   6.160   9.569  1.00  3.24           C
ATOM   1054  C   TRP A 516      17.952   5.169  12.003  1.00  4.43           C
ATOM   1055  O   TRP A 516      17.926   6.353  11.702  1.00  3.37           O
ATOM   1056  N   ILE A 517      17.666   4.740  13.200  1.00  3.57           N
ATOM   1057  CA  ILE A 517      17.185   5.585  14.267  1.00  4.13           C
ATOM   1058  CB  ILE A 517      16.858   4.736  15.545  1.00  3.53           C
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ATOM   1059  CG1 ILE A 517      15.951   5.447  16.492  1.00  3.79           C
ATOM   1060  CD1 ILE A 517      14.834   6.161  15.859  1.00  2.00           C
ATOM   1061  CG2 ILE A 517      18.075   4.328  16.251  1.00  2.00           C
ATOM   1062  C   ILE A 517      18.212   6.609  14.585  1.00  6.38           C
ATOM   1063  O   ILE A 517      17.848   7.674  15.015  1.00  8.32           O
ATOM   1064  N   LEU A 518      19.497   6.317  14.379  1.00  7.30           N
ATOM   1065  CA  LEU A 518      20.514   7.275  14.739  1.00  6.90           C
ATOM   1066  CB  LEU A 518      21.899   6.677  14.639  1.00  7.32           C
ATOM   1067  CG  LEU A 518      22.196   5.522  15.627  1.00  8.35           C
ATOM   1068  CD1 LEU A 518      23.684   5.126  15.647  1.00  2.50           C
ATOM   1069  CD2 LEU A 518      21.682   5.833  16.977  1.00  5.08           C
ATOM   1070  C   LEU A 518      20.392   8.434  13.817  1.00  7.74           C
ATOM   1071  O   LEU A 518      20.237   9.526  14.269  1.00  7.58           O
ATOM   1072  N   ASN A 519      20.409   8.196  12.511  1.00  9.38           N
ATOM   1073  CA  ASN A 519      20.366   9.250  11.525  1.00 11.13           C
ATOM   1074  CB  ASN A 519      20.446   8.593  10.162  1.00 13.71           C
ATOM   1075  CG  ASN A 519      21.098   9.498   9.094  1.00 23.00           C
ATOM   1076  OD1 ASN A 519      22.350   9.727   9.100  1.00 30.67           O
ATOM   1077  ND2 ASN A 519      20.268  10.018   8.169  1.00 22.67           N
ATOM   1078  C   ASN A 519      19.046  10.037  11.701  1.00 10.46           C
ATOM   1079  O   ASN A 519      19.004  11.240  11.786  1.00 11.31           O
ATOM   1080  N   VAL A 520      17.949   9.344  11.879  1.00  9.13           N
ATOM   1081  CA  VAL A 520      16.709  10.025  12.095  1.00  8.53           C
ATOM   1082  CB  VAL A 520      15.620   8.949  12.461  1.00 10.43           C
ATOM   1083  CG1 VAL A 520      14.333   9.580  12.952  1.00 10.55           C
ATOM   1084  CG2 VAL A 520      15.317   8.122  11.201  1.00 13.73           C
ATOM   1085  C   VAL A 520      16.771  11.115  13.191  1.00  6.90           C
ATOM   1086  O   VAL A 520      16.164  12.190  13.044  1.00  3.70           O
ATOM   1087  N   LEU A 521      17.443  10.792  14.314  1.00  5.11           N
ATOM   1088  CA  LEU A 521      17.522  11.711  15.441  1.00  4.30           C
ATOM   1089  CB  LEU A 521      17.357  10.946  16.736  1.00  4.31           C
ATOM   1090  CG  LEU A 521      16.071  10.118  16.854  1.00  7.22           C
ATOM   1091  CD1 LEU A 521      15.983   9.289  18.178  1.00  7.33           C
ATOM   1092  CD2 LEU A 521      14.901  11.002  16.779  1.00  7.22           C
ATOM   1093  C   LEU A 521      18.823  12.577  15.474  1.00  4.02           C
ATOM   1094  O   LEU A 521      19.011  13.401  16.394  1.00  2.26           O
ATOM   1095  N   ASN A 522      19.688  12.407  14.458  1.00  2.73           N
ATOM   1096  CA  ASN A 522      20.955  13.075  14.488  1.00  2.77           C
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ATOM   1097  CB  ASN A 522      20.752  14.599  14.324  1.00  3.11           C
ATOM   1098  CG  ASN A 522      21.989  15.287  13.874  1.00  2.00           C
ATOM   1099  OD1 ASN A 522      22.890  14.661  13.307  1.00  5.97           O
ATOM   1100  ND2 ASN A 522      22.010  16.571  13.998  1.00  2.15           N
ATOM   1101  C   ASN A 522      21.802  12.771  15.773  1.00  2.00           C
ATOM   1102  O   ASN A 522      22.511  13.624  16.287  1.00  3.48           O
ATOM   1103  N   LEU A 523      21.783  11.539  16.200  1.00  2.26           N
ATOM   1104  CA  LEU A 523      22.438  11.082  17.427  1.00  3.51           C
ATOM   1105  CB  LEU A 523      21.428  10.220  18.177  1.00  2.69           C
ATOM   1106  CG  LEU A 523      21.532   9.986  19.629  1.00  3.52           C
ATOM   1107  CD1 LEU A 523      20.849   8.528  19.873  1.00  3.71           C
ATOM   1108  CD2 LEU A 523      22.971   9.957  19.828  1.00 12.53           C
ATOM   1109  C   LEU A 523      23.614  10.191  17.090  1.00  3.88           C
ATOM   1110  O   LEU A 523      23.485   9.219  16.297  1.00  4.01           O
ATOM   1111  N   LYS A 524      24.746  10.461  17.716  1.00  2.74           N
ATOM   1112  CA  LYS A 524      25.903   9.601  17.474  1.00  2.84           C
ATOM   1113  CB  LYS A 524      27.149  10.334  17.836  1.00  2.00           C
ATOM   1114  CG  LYS A 524      27.149  11.724  17.147  1.00  2.00           C
ATOM   1115  CD  LYS A 524      27.457  11.584  15.679  1.00  2.78           C
ATOM   1116  CE  LYS A 524      27.418  12.949  14.980  1.00  7.61           C
ATOM   1117  NZ  LYS A 524      27.359  12.847  13.479  1.00 11.33           N
ATOM   1118  C   LYS A 524      25.885   8.202  18.109  1.00  3.34           C
ATOM   1119  O   LYS A 524      25.280   7.964  19.167  1.00  3.82           O
ATOM   1120  N   ALA A 525      26.506   7.261  17.441  1.00  3.11           N
ATOM   1121  CA  ALA A 525      26.598   5.910  17.958  1.00  3.88           C
ATOM   1122  CB  ALA A 525      27.316   5.015  16.961  1.00  2.69           C
ATOM   1123  C   ALA A 525      27.273   5.816  19.369  1.00  5.48           C
ATOM   1124  O   ALA A 525      26.858   5.010  20.264  1.00  5.29           O
ATOM   1125  N   PHE A 526      28.325   6.610  19.571  1.00  5.00           N
ATOM   1126  CA  PHE A 526      29.027   6.484  20.806  1.00  5.18           C
ATOM   1127  CB  PHE A 526      30.353   7.286  20.777  1.00  5.32           C
ATOM   1128  CG  PHE A 526      31.143   7.206  22.059  1.00  6.17           C
ATOM   1129  CD1 PHE A 526      31.814   6.036  22.377  1.00  2.97           C
ATOM   1130  CE1 PHE A 526      32.505   5.936  23.581  1.00  3.73           C
ATOM   1131  CZ  PHE A 526      32.494   7.010  24.568  1.00  2.63           C
ATOM   1132  CE2 PHE A 526      31.822   8.187  24.280  1.00  3.05           C
ATOM   1133  CD2 PHE A 526      31.111   8.274  23.014  1.00  5.63           C
ATOM   1134  C   PHE A 526      28.109   6.884  21.983  1.00  5.59           C
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ATOM   1135  O   PHE A 526      28.240   6.292  23.098  1.00  4.24           O
ATOM   1136  N   ASP A 527      27.251   7.911  21.773  1.00  4.53           N
ATOM   1137  CA  ASP A 527      26.313   8.356  22.846  1.00  4.18           C
ATOM   1138  CB  ASP A 527      25.701   9.662  22.496  1.00  3.20           C
ATOM   1139  CG  ASP A 527      26.718  10.775  22.359  1.00  5.73           C
ATOM   1140  OD1 ASP A 527      27.665  10.941  23.205  1.00  6.84           O
ATOM   1141  OD2 ASP A 527      26.598  11.619  21.454  1.00  9.35           O
ATOM   1142  C   ASP A 527      25.187   7.375  23.150  1.00  4.67           C
ATOM   1143  O   ASP A 527      24.739   7.280  24.286  1.00  6.22           O
ATOM   1144  N   PHE A 528      24.737   6.649  22.136  1.00  4.38           N
ATOM   1145  CA  PHE A 528      23.658   5.687  22.227  1.00  6.14           C
ATOM   1146  CB  PHE A 528      23.358   5.130  20.803  1.00  7.25           C
ATOM   1147  CG  PHE A 528      22.132   4.250  20.713  1.00  8.05           C
ATOM   1148  CD1 PHE A 528      20.924   4.782  20.311  1.00  6.37           C
ATOM   1149  CE1 PHE A 528      19.799   3.975  20.164  1.00  7.19           C
ATOM   1150  CZ  PHE A 528      19.874   2.577  20.441  1.00  5.82           C
ATOM   1151  CE2 PHE A 528      21.068   2.038  20.784  1.00  5.09           C
ATOM   1152  CD2 PHE A 528      22.218   2.866  20.917  1.00  7.19           C
ATOM   1153  C   PHE A 528      24.105   4.578  23.126  1.00  6.06           C
ATOM   1154  O   PHE A 528      23.425   4.228  24.084  1.00  6.25           O
ATOM   1155  N   TYR A 529      25.289   4.066  22.816  1.00  6.43           N
ATOM   1156  CA  TYR A 529      25.938   3.007  23.562  1.00  6.94           C
ATOM   1157  CB  TYR A 529      27.387   2.762  23.011  1.00  7.10           C
ATOM   1158  CG  TYR A 529      28.385   2.752  24.090  1.00  7.19           C
ATOM   1159  CD1 TYR A 529      28.491   1.668  24.986  1.00 11.52           C
ATOM   1160  CE1 TYR A 529      29.389   1.711  26.088  1.00 10.35           C
ATOM   1161  CZ  TYR A 529      30.151   2.858  26.287  1.00 13.78           C
ATOM   1162  OH  TYR A 529      31.044   2.977  27.345  1.00 19.36           O
ATOM   1163  CE2 TYR A 529      30.068   3.915  25.405  1.00 11.15           C
ATOM   1164  CD2 TYR A 529      29.151   3.849  24.312  1.00  8.73           C
ATOM   1165  C   TYR A 529      25.935   3.312  25.069  1.00  7.03           C
ATOM   1166  O   TYR A 529      25.690   2.457  25.848  1.00  6.96           O
ATOM   1167  N   LYS A 530      26.238   4.532  25.478  1.00  7.01           N
ATOM   1168  CA  LYS A 530      26.239   4.848  26.893  1.00  7.93           C
ATOM   1169  CB  LYS A 530      26.554   6.323  27.075  1.00  8.59           C
ATOM   1170  CG  LYS A 530      27.919   6.736  26.434  1.00 12.70           C
ATOM   1171  CD  LYS A 530      28.593   7.898  27.168  1.00 15.96           C
ATOM   1172  CE  LYS A 530      27.983   9.237  26.949  1.00 16.66           C
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ATOM   1173  NZ  LYS A 530      28.524  10.243  27.977  1.00 21.28           N
ATOM   1174  C   LYS A 530      24.930   4.531  27.635  1.00  7.04           C
ATOM   1175  O   LYS A 530      24.894   4.454  28.847  1.00  6.48           O
ATOM   1176  N   VAL A 531      23.871   4.272  26.892  1.00  6.56           N
ATOM   1177  CA  VAL A 531      22.577   4.052  27.500  1.00  6.44           C
ATOM   1178  CB  VAL A 531      21.516   4.971  26.840  1.00  7.07           C
ATOM   1179  CG1 VAL A 531      20.343   4.227  26.381  1.00  6.11           C
ATOM   1180  CG2 VAL A 531      21.123   6.035  27.787  1.00  5.82           C
ATOM   1181  C   VAL A 531      22.123   2.598  27.510  1.00  6.24           C
ATOM   1182  O   VAL A 531      21.231   2.236  28.299  1.00  5.96           O
ATOM   1183  N   ILE A 532      22.781   1.762  26.700  1.00  5.58           N
ATOM   1184  CA  ILE A 532      22.429   0.353  26.549  1.00  5.19           C
ATOM   1185  CB  ILE A 532      23.238  -0.250  25.456  1.00  4.47           C
ATOM   1186  CG1 ILE A 532      22.889   0.411  24.083  1.00  4.56           C
ATOM   1187  CD1 ILE A 532      23.696  -0.133  22.877  1.00  2.00           C
ATOM   1188  CG2 ILE A 532      22.953  -1.674  25.387  1.00  4.32           C
ATOM   1189  C   ILE A 532      22.488  -0.511  27.837  1.00  6.67           C
ATOM   1190  O   ILE A 532      21.454  -1.055  28.285  1.00  7.52           O
ATOM   1191  N   GLU A 533      23.629  -0.609  28.507  1.00  6.39           N
ATOM   1192  CA  GLU A 533      23.677  -1.499  29.691  1.00  6.52           C
ATOM   1193  CB  GLU A 533      25.067  -1.550  30.317  1.00  6.68           C
ATOM   1194  CG  GLU A 533      25.272  -2.671  31.320  1.00 11.17           C
ATOM   1195  CD  GLU A 533      26.738  -2.845  31.725  1.00 16.80           C
ATOM   1196  OE1 GLU A 533      27.562  -2.996  30.800  1.00 19.44           O
ATOM   1197  OE2 GLU A 533      27.094  -2.828  32.935  1.00 16.76           O
ATOM   1198  C   GLU A 533      22.683  -1.098  30.776  1.00  6.18           C
ATOM   1199  O   GLU A 533      22.077  -1.966  31.395  1.00  6.74           O
ATOM   1200  N   SER A 534      22.497   0.211  30.998  1.00  5.64           N
ATOM   1201  CA  SER A 534      21.585   0.679  32.030  1.00  4.84           C
ATOM   1202  CB  SER A 534      21.769   2.187  32.279  1.00  4.45           C
ATOM   1203  OG  SER A 534      23.070   2.400  32.781  1.00  5.10           O
ATOM   1204  C   SER A 534      20.139   0.394  31.664  1.00  5.13           C
ATOM   1205  O   SER A 534      19.329   0.055  32.511  1.00  4.57           O
ATOM   1206  N   PHE A 535      19.828   0.544  30.377  1.00  5.26           N
ATOM   1207  CA  PHE A 535      18.497   0.293  29.885  1.00  4.73           C
ATOM   1208  CB  PHE A 535      18.453   0.649  28.394  1.00  4.00           C
ATOM   1209  CG  PHE A 535      17.077   0.596  27.794  1.00  5.70           C
ATOM   1210  CD1 PHE A 535      16.418  -0.623  27.601  1.00  6.27           C
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ATOM   1211  CE1 PHE A 535      15.157  -0.682  27.055  1.00  4.58           C
ATOM   1212  CZ  PHE A 535      14.532   0.449  26.709  1.00  4.63           C
ATOM   1213  CE2 PHE A 535      15.156   1.683  26.907  1.00  7.49           C
ATOM   1214  CD2 PHE A 535      16.430   1.759  27.424  1.00  6.81           C
ATOM   1215  C   PHE A 535      18.138  -1.186  30.165  1.00  4.51           C
ATOM   1216  O   PHE A 535      17.052  -1.477  30.621  1.00  3.71           O
ATOM   1217  N   ILE A 536      19.077  -2.093  29.898  1.00  4.10           N
ATOM   1218  CA  ILE A 536      18.874  -3.495  30.168  1.00  4.80           C
ATOM   1219  CB  ILE A 536      20.025  -4.347  29.670  1.00  4.93           C
ATOM   1220  CG1 ILE A 536      20.014  -4.414  28.161  1.00  2.00           C
ATOM   1221  CD1 ILE A 536      21.367  -4.726  27.637  1.00  2.00           C
ATOM   1222  CG2 ILE A 536      19.894  -5.757  30.160  1.00  2.46           C
ATOM   1223  C   ILE A 536      18.664  -3.836  31.638  1.00  6.22           C
ATOM   1224  O   ILE A 536      17.956  -4.791  31.910  1.00  7.20           O
ATOM   1225  N   LYS A 537      19.245  -3.082  32.571  1.00  7.13           N
ATOM   1226  CA  LYS A 537      19.039  -3.360  34.010  1.00  7.81           C
ATOM   1227  CB  LYS A 537      20.210  -2.954  34.920  1.00  8.38           C
ATOM   1228  CG  LYS A 537      21.589  -3.503  34.638  1.00 11.82           C
ATOM   1229  CD  LYS A 537      22.582  -2.777  35.588  1.00 20.54           C
ATOM   1230  CE  LYS A 537      24.072  -2.945  35.157  1.00 26.43           C
ATOM   1231  NZ  LYS A 537      25.029  -2.886  36.319  1.00 26.23           N
ATOM   1232  C   LYS A 537      17.853  -2.665  34.540  1.00  6.91           C
ATOM   1233  O   LYS A 537      17.360  -3.015  35.570  1.00  7.82           O
ATOM   1234  N   ALA A 538      17.402  -1.626  33.873  1.00  6.92           N
ATOM   1235  CA  ALA A 538      16.250  -0.901  34.370  1.00  5.49           C
ATOM   1236  CB  ALA A 538      16.297   0.503  33.897  1.00  4.12           C
ATOM   1237  C   ALA A 538      14.926  -1.537  33.966  1.00  6.38           C
ATOM   1238  O   ALA A 538      13.957  -1.305  34.626  1.00  6.33           O
ATOM   1239  N   GLU A 539      14.879  -2.296  32.870  1.00  7.70           N
ATOM   1240  CA  GLU A 539      13.655  -2.885  32.354  1.00  8.69           C
ATOM   1241  CB  GLU A 539      13.550  -2.681  30.821  1.00 10.15           C
ATOM   1242  CG  GLU A 539      12.180  -3.034  30.261  1.00 10.13           C
ATOM   1243  CD  GLU A 539      11.089  -2.643  31.275  1.00 14.92           C
ATOM   1244  OE1 GLU A 539      10.984  -1.404  31.629  1.00 14.92           O
ATOM   1245  OE2 GLU A 539      10.377  -3.560  31.747  1.00 11.46           O
ATOM   1246  C   GLU A 539      13.662  -4.373  32.559  1.00  9.87           C
ATOM   1247  O   GLU A 539      14.241  -5.145  31.725  1.00 11.40           O
ATOM   1248  N   GLY A 540      12.982  -4.820  33.599  1.00  8.74           N
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ATOM   1249  CA  GLY A 540      12.926  -6.240  33.832  1.00  8.45           C
ATOM   1250  C   GLY A 540      12.031  -7.044  32.889  1.00  8.50           C
ATOM   1251  O   GLY A 540      12.013  -8.249  32.981  1.00  8.50           O
ATOM   1252  N   ASN A 541      11.296  -6.412  31.987  1.00  8.51           N
ATOM   1253  CA  ASN A 541      10.420  -7.177  31.125  1.00  9.67           C
ATOM   1254  CB  ASN A 541       9.033  -6.558  31.090  1.00  9.96           C
ATOM   1255  CG  ASN A 541       8.315  -6.684  32.421  1.00 12.87           C
ATOM   1256  OD1 ASN A 541       7.510  -7.576  32.607  1.00 15.20           O
ATOM   1257  ND2 ASN A 541       8.603  -5.782  33.346  1.00 11.13           N
ATOM   1258  C   ASN A 541      10.911  -7.378  29.706  1.00  9.56           C
ATOM   1259  O   ASN A 541      10.126  -7.663  28.823  1.00 10.01           O
ATOM   1260  N   LEU A 542      12.207  -7.232  29.472  1.00  9.76           N
ATOM   1261  CA  LEU A 542      12.717  -7.373  28.095  1.00  9.10           C
ATOM   1262  CB  LEU A 542      14.075  -6.684  27.941  1.00  8.09           C
ATOM   1263  CG  LEU A 542      14.095  -5.179  27.973  1.00  8.97           C
ATOM   1264  CD1 LEU A 542      15.492  -4.668  28.053  1.00  9.22           C
ATOM   1265  CD2 LEU A 542      13.403  -4.622  26.759  1.00  9.80           C
ATOM   1266  C   LEU A 542      12.852  -8.848  27.746  1.00  8.30           C
ATOM   1267  O   LEU A 542      13.338  -9.615  28.540  1.00  8.47           O
ATOM   1268  N   THR A 543      12.463  -9.247  26.547  1.00  8.14           N
ATOM   1269  CA  THR A 543      12.631 -10.650  26.147  1.00  7.80           C
ATOM   1270  CB  THR A 543      11.922 -10.978  24.831  1.00  6.70           C
ATOM   1271  OG1 THR A 543      12.469 -10.196  23.781  1.00  4.89           O
ATOM   1272  CG2 THR A 543      10.487 -10.605  24.853  1.00  7.19           C
ATOM   1273  C   THR A 543      14.089 -11.004  25.939  1.00  9.04           C
ATOM   1274  O   THR A 543      14.967 -10.139  25.938  1.00  9.69           O
ATOM   1275  N   ARG A 544      14.325 -12.283  25.690  1.00  9.66           N
ATOM   1276  CA  ARG A 544      15.657 -12.785  25.472  1.00 10.93           C
ATOM   1277  CB  ARG A 544      15.645 -14.329  25.540  1.00 11.59           C
ATOM   1278  CG  ARG A 544      16.929 -15.067  25.014  1.00 10.88           C
ATOM   1279  CD  ARG A 544      16.848 -16.618  25.167  1.00 14.78           C
ATOM   1280  NE  ARG A 544      15.749 -17.233  24.413  1.00 13.02           N
ATOM   1281  CZ  ARG A 544      15.747 -17.391  23.074  1.00 18.91           C
ATOM   1282  NH1 ARG A 544      16.775 -16.942  22.355  1.00 23.09           N
ATOM   1283  NH2 ARG A 544      14.719 -17.965  22.422  1.00 17.48           N
ATOM   1284  C   ARG A 544      16.117 -12.289  24.106  1.00 11.05           C
ATOM   1285  O   ARG A 544      17.262 -11.979  23.932  1.00 10.33           O
ATOM   1286  N   GLU A 545      15.186 -12.211  23.167  1.00 11.63           N
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ATOM   1287  CA  GLU A 545      15.455 -11.772  21.819  1.00 13.95           C
ATOM   1288  CB  GLU A 545      14.246 -12.016  20.946  1.00 13.76           C
ATOM   1289  CG  GLU A 545      13.860 -13.495  20.890  1.00 21.85           C
ATOM   1290  CD  GLU A 545      13.715 -14.208  22.292  1.00 28.21           C
ATOM   1291  OE1 GLU A 545      13.028 -13.699  23.251  1.00 22.99           O
ATOM   1292  OE2 GLU A 545      14.307 -15.320  22.427  1.00 29.40           O
ATOM   1293  C   GLU A 545      15.772 -10.298  21.757  1.00 14.02           C
ATOM   1294  O   GLU A 545      16.548  -9.871  20.921  1.00 14.84           O
ATOM   1295  N   MET A 546      15.154  -9.530  22.646  1.00 13.93           N
ATOM   1296  CA  MET A 546      15.330  -8.086  22.725  1.00 13.00           C
ATOM   1297  CB  MET A 546      14.159  -7.478  23.524  1.00 13.31           C
ATOM   1298  CG  MET A 546      13.948  -5.997  23.287  1.00 19.54           C
ATOM   1299  SD  MET A 546      13.855  -5.454  21.439  1.00 29.26           S
ATOM   1300  CE  MET A 546      15.547  -5.068  21.117  1.00 21.36           C
ATOM   1301  C   MET A 546      16.706  -7.727  23.314  1.00 10.12           C
ATOM   1302  O   MET A 546      17.354  -6.831  22.867  1.00  7.74           O
ATOM   1303  N   ILE A 547      17.154  -8.475  24.313  1.00  9.83           N
ATOM   1304  CA  ILE A 547      18.459  -8.235  24.923  1.00  8.79           C
ATOM   1305  CB  ILE A 547      18.601  -9.080  26.159  1.00  7.97           C
ATOM   1306  CG1 ILE A 547      17.582  -8.632  27.190  1.00  7.88           C
ATOM   1307  CD1 ILE A 547      17.608  -9.481  28.521  1.00  7.89           C
ATOM   1308  CG2 ILE A 547      19.986  -8.952  26.827  1.00  8.85           C
ATOM   1309  C   ILE A 547      19.476  -8.603  23.875  1.00  8.59           C
ATOM   1310  O   ILE A 547      20.432  -7.911  23.585  1.00  9.01           O
ATOM   1311  N   LYS A 548      19.203  -9.683  23.224  1.00  8.48           N
ATOM   1312  CA  LYS A 548      20.060 -10.106  22.157  1.00  8.58           C
ATOM   1313  CB  LYS A 548      19.527 -11.417  21.580  1.00  8.46           C
ATOM   1314  CG  LYS A 548      20.646 -12.366  21.115  1.00 14.13           C
ATOM   1315  CD  LYS A 548      20.837 -13.592  22.053  1.00 20.90           C
ATOM   1316  CE  LYS A 548      21.254 -13.189  23.487  1.00 24.85           C
ATOM   1317  NZ  LYS A 548      21.477 -14.338  24.469  1.00 25.80           N
ATOM   1318  C   LYS A 548      20.211  -9.024  21.088  1.00  7.39           C
ATOM   1319  O   LYS A 548      21.321  -8.759  20.627  1.00  7.65           O
ATOM   1320  N   HIS A 549      19.100  -8.402  20.689  1.00  5.99           N
ATOM   1321  CA  HIS A 549      19.118  -7.426  19.629  1.00  3.72           C
ATOM   1322  CB  HIS A 549      17.703  -7.050  19.213  1.00  2.50           C
ATOM   1323  CG  HIS A 549      17.656  -5.973  18.172  1.00  4.11           C
ATOM   1324  ND1 HIS A 549      18.258  -6.102  16.932  1.00  2.57           N
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ATOM   1325  CE1 HIS A 549      18.083  -4.979  16.253  1.00  2.00           C
ATOM   1326  NE2 HIS A 549      17.394  -4.134  17.003  1.00  2.00           N
ATOM   1327  CD2 HIS A 549      17.121  -4.725  18.206  1.00  2.00           C
ATOM   1328  C   HIS A 549      19.919  -6.219  20.099  1.00  4.21           C
ATOM   1329  O   HIS A 549      20.773  -5.673  19.357  1.00  2.85           O
ATOM   1330  N   LEU A 550      19.698  -5.856  21.366  1.00  4.44           N
ATOM   1331  CA  LEU A 550      20.395  -4.711  21.962  1.00  5.58           C
ATOM   1332  CB  LEU A 550      19.851  -4.379  23.369  1.00  4.96           C
ATOM   1333  CG  LEU A 550      18.486  -3.698  23.396  1.00  6.21           C
ATOM   1334  CD1 LEU A 550      18.194  -3.255  24.820  1.00  9.90           C
ATOM   1335  CD2 LEU A 550      18.512  -2.473  22.485  1.00  8.87           C
ATOM   1336  C   LEU A 550      21.912  -4.937  21.991  1.00  5.86           C
ATOM   1337  O   LEU A 550      22.693  -4.018  21.757  1.00  5.64           O
ATOM   1338  N   GLU A 551      22.318  -6.167  22.289  1.00  5.89           N
ATOM   1339  CA  GLU A 551      23.714  -6.493  22.297  1.00  7.35           C
ATOM   1340  CB  GLU A 551      23.897  -7.847  22.907  1.00  7.43           C
ATOM   1341  CG  GLU A 551      25.312  -8.358  22.922  1.00 11.11           C
ATOM   1342  CD  GLU A 551      25.376  -9.858  23.196  1.00 12.97           C
ATOM   1343  OE1 GLU A 551      25.783 -10.217  24.325  1.00 13.82           O
ATOM   1344  OE2 GLU A 551      25.015 -10.655  22.287  1.00 12.23           O
ATOM   1345  C   GLU A 551      24.347  -6.418  20.897  1.00  7.94           C
ATOM   1346  O   GLU A 551      25.475  -5.935  20.720  1.00  8.12           O
ATOM   1347  N   ARG A 552      23.616  -6.849  19.888  1.00  8.62           N
ATOM   1348  CA  ARG A 552      24.128  -6.750  18.529  1.00 10.18           C
ATOM   1349  CB  ARG A 552      23.144  -7.403  17.595  1.00 12.41           C
ATOM   1350  CG  ARG A 552      23.649  -7.583  16.190  1.00 20.85           C
ATOM   1351  CD  ARG A 552      24.954  -8.372  16.069  1.00 27.00           C
ATOM   1352  NE  ARG A 552      25.734  -7.818  14.969  1.00 30.08           N
ATOM   1353  CZ  ARG A 552      27.060  -7.851  14.950  1.00 34.49           C
ATOM   1354  NH1 ARG A 552      27.664  -8.435  15.999  1.00 30.27           N
ATOM   1355  NH2 ARG A 552      27.773  -7.319  13.901  1.00 34.69           N
ATOM   1356  C   ARG A 552      24.352  -5.292  18.076  1.00  9.36           C
ATOM   1357  O   ARG A 552      25.304  -5.020  17.357  1.00  9.30           O
ATOM   1358  N   CYS A 553      23.467  -4.381  18.496  1.00  7.47           N
ATOM   1359  CA  CYS A 553      23.615  -2.972  18.243  1.00  7.51           C
ATOM   1360  CB  CYS A 553      22.387  -2.146  18.736  1.00  7.23           C
ATOM   1361  SG  CYS A 553      20.754  -2.427  17.964  1.00  7.13           S
ATOM   1362  C   CYS A 553      24.890  -2.480  18.971  1.00  7.59           C
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ATOM   1363  O   CYS A 553      25.704  -1.706  18.435  1.00  7.17           O
ATOM   1364  N   GLU A 554      25.084  -2.959  20.180  1.00  6.68           N
ATOM   1365  CA  GLU A 554      26.265  -2.557  20.905  1.00  8.06           C
ATOM   1366  CB  GLU A 554      26.211  -3.111  22.321  1.00  7.22           C
ATOM   1367  CG  GLU A 554      27.140  -2.424  23.280  1.00  5.98           C
ATOM   1368  CD  GLU A 554      26.917  -2.886  24.688  1.00 11.28           C
ATOM   1369  OE1 GLU A 554      26.704  -4.112  24.903  1.00 15.10           O
ATOM   1370  OE2 GLU A 554      26.930  -2.034  25.602  1.00 14.58           O
ATOM   1371  C   GLU A 554      27.576  -2.999  20.274  1.00  8.25           C
ATOM   1372  O   GLU A 554      28.592  -2.329  20.318  1.00  9.11           O
ATOM   1373  N   HIS A 555      27.561  -4.184  19.737  1.00  8.65           N
ATOM   1374  CA  HIS A 555      28.736  -4.736  19.112  1.00  7.90           C
ATOM   1375  CB  HIS A 555      28.487  -6.229  18.855  1.00  6.62           C
ATOM   1376  CG  HIS A 555      28.603  -7.083  20.083  1.00  4.39           C
ATOM   1377  ND1 HIS A 555      28.242  -8.418  20.099  1.00  2.00           N
ATOM   1378  CE1 HIS A 555      28.523  -8.929  21.283  1.00  2.00           C
ATOM   1379  NE2 HIS A 555      29.024  -7.971  22.050  1.00  2.00           N
ATOM   1380  CD2 HIS A 555      29.094  -6.808  21.319  1.00  2.05           C
ATOM   1381  C   HIS A 555      29.067  -3.985  17.817  1.00  8.31           C
ATOM   1382  O   HIS A 555      30.235  -3.850  17.416  1.00  8.87           O
ATOM   1383  N   ARG A 556      28.046  -3.483  17.145  1.00  7.61           N
ATOM   1384  CA  ARG A 556      28.312  -2.784  15.910  1.00  7.11           C
ATOM   1385  CB  ARG A 556      27.068  -2.745  15.032  1.00  7.58           C
ATOM   1386  CG  ARG A 556      26.830  -4.086  14.419  1.00 12.81           C
ATOM   1387  CD  ARG A 556      25.422  -4.476  14.251  1.00 19.23           C
ATOM   1388  NE  ARG A 556      24.910  -3.879  13.043  1.00 22.82           N
ATOM   1389  CZ  ARG A 556      23.632  -3.796  12.766  1.00 25.22           C
ATOM   1390  NH1 ARG A 556      22.735  -4.276  13.647  1.00 23.17           N
ATOM   1391  NH2 ARG A 556      23.255  -3.226  11.619  1.00 23.51           N
ATOM   1392  C   ARG A 556      28.790  -1.417  16.218  1.00  5.89           C
ATOM   1393  O   ARG A 556      29.447  -0.835  15.400  1.00  6.78           O
ATOM   1394  N   ILE A 557      28.480  -0.890  17.404  1.00  4.95           N
ATOM   1395  CA  ILE A 557      28.975   0.438  17.777  1.00  3.96           C
ATOM   1396  CB  ILE A 557      28.195   0.966  18.957  1.00  4.35           C
ATOM   1397  CG1 ILE A 557      26.718   1.166  18.578  1.00  3.64           C
ATOM   1398  CD1 ILE A 557      25.860   1.516  19.797  1.00  2.00           C
ATOM   1399  CG2 ILE A 557      28.762   2.324  19.538  1.00  2.19           C
ATOM   1400  C   ILE A 557      30.462   0.279  18.067  1.00  5.06           C
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ATOM   1401  O   ILE A 557      31.301   1.023  17.582  1.00  3.84           O
ATOM   1402  N   MET A 558      30.774  -0.732  18.862  1.00  6.34           N
ATOM   1403  CA  MET A 558     32.137  -1.072  19.214  1.00  7.02           C
ATOM   1404  CB  MET A 558     32.147  -2.170  20.277  1.00  7.34           C
ATOM   1405  CG  MET A 558     31.501  -1.673  21.619  1.00 12.35           C
ATOM   1406  SD  MET A 558     31.502  -2.949  22.900  1.00 17.81           S
ATOM   1407  CE  MET A 558     30.101  -3.923  22.556  1.00 14.43           C
ATOM   1408  C   MET A 558     33.009  -1.491  18.054  1.00  5.34           C
ATOM   1409  O   MET A 558     34.222  -1.284  18.091  1.00  4.60           O
ATOM   1410  N   GLU A 559     32.417  -2.102  17.040  1.00  3.43           N
ATOM   1411  CA  GLU A 559     33.269  -2.609  15.983  1.00  2.79           C
ATOM   1412  CB  GLU A 559     32.673  -3.807  15.250  1.00  3.49           C
ATOM   1413  CG  GLU A 559     31.360  -3.495  14.562  1.00  6.17           C
ATOM   1414  CD  GLU A 559     30.720  -4.665  13.825  1.00  9.46           C
ATOM   1415  OE1 GLU A 559     30.780  -5.820  14.299  1.00  6.19           O
ATOM   1416  OE2 GLU A 559     30.122  -4.376  12.742  1.00 13.37           O
ATOM   1417  C   GLU A 559     33.642  -1.514  15.017  1.00  2.46           C
ATOM   1418  O   GLU A 559     34.777  -1.515  14.553  1.00  3.03           O
ATOM   1419  N   SER A 560     32.722  -0.585  14.708  1.00  2.00           N
ATOM   1420  CA  SER A 560     32.999   0.509  13.765  1.00  2.00           C
ATOM   1421  CB  SER A 560     32.848   0.074  12.287  1.00  2.00           C
ATOM   1422  OG  SER A 560     31.566  -0.370  11.966  1.00  2.00           O
ATOM   1423  C   SER A 560     32.339   1.845  13.960  1.00  2.00           C
ATOM   1424  O   SER A 560     33.008   2.816  14.009  1.00  2.06           O
ATOM   1425  N   LEU A 561     31.020   1.902  14.097  1.00  2.00           N
ATOM   1426  CA  LEU A 561     30.323   3.156  14.220  1.00  2.20           C
ATOM   1427  CB  LEU A 561     28.835   2.896  14.518  1.00  2.33           C
ATOM   1428  CG  LEU A 561     27.969   2.019  13.593  1.00  4.31           C
ATOM   1429  CD1 LEU A 561     26.528   1.785  14.215  1.00  2.00           C
ATOM   1430  CD2 LEU A 561     27.927   2.524  12.106  1.00  2.00           C
ATOM   1431  C   LEU A 561     30.959   4.193  15.219  1.00  2.00           C
ATOM   1432  O   LEU A 561     31.119   5.361  14.911  1.00  2.00           O
ATOM   1433  N   ALA A 562     31.326   3.756  16.393  1.00  2.00           N
ATOM   1434  CA  ALA A 562     31.879   4.693  17.354  1.00  2.83           C
ATOM   1435  CB  ALA A 562     31.979   4.095  18.810  1.00  2.00           C
ATOM   1436  C   ALA A 562     33.259   5.109  16.884  1.00  3.11           C
ATOM   1437  O   ALA A 562     33.863   5.921  17.530  1.00  3.18           O
ATOM   1438  N   TRP A 563     33.768   4.535  15.806  1.00  2.21           N
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ATOM	1439	CA	TRP	A	563	35.073	4.973	15.316	1.00	3.35	C
ATOM	1440	CB	TRP	A	563	36.036	3.777	15.101	1.00	2.70	C
ATOM	1441	CG	TRP	A	563	36.208	2.881	16.308	1.00	3.50	C
ATOM	1442	CD1	TRP	A	563	35.434	1.796	16.638	1.00	4.08	C
ATOM	1443	NE1	TRP	A	563	35.881	1.214	17.793	1.00	2.00	N
ATOM	1444	CE2	TRP	A	563	36.974	1.908	18.231	1.00	2.92	C
ATOM	1445	CD2	TRP	A	563	37.222	2.948	17.292	1.00	2.00	C
ATOM	1446	CE3	TRP	A	563	38.273	3.804	17.524	1.00	2.65	C
ATOM	1447	CZ3	TRP	A	563	39.083	3.601	18.648	1.00	3.77	C
ATOM	1448	CH2	TRP	A	563	38.839	2.532	19.547	1.00	2.00	C
ATOM	1449	CZ2	TRP	A	563	37.786	1.694	19.378	1.00	2.00	C
ATOM	1450	C	TRP	A	563	34.969	5.825	14.016	1.00	3.80	C
ATOM	1451	O	TRP	A	563	35.925	6.044	13.306	1.00	2.92	O
ATOM	1452	N	LEU	A	564	33.777	6.253	13.660	1.00	4.71	N
ATOM	1453	CA	LEU	A	564	33.712	7.145	12.484	1.00	5.58	C
ATOM	1454	CB	LEU	A	564	32.264	7.290	11.965	1.00	4.26	C
ATOM	1455	CG	LEU	A	564	31.566	6.068	11.390	1.00	4.77	C
ATOM	1456	CD1	LEU	A	564	30.004	6.356	11.192	1.00	3.32	C
ATOM	1457	CD2	LEU	A	564	32.200	5.550	10.050	1.00	2.00	C
ATOM	1458	C	LEU	A	564	34.290	8.532	12.858	1.00	4.78	C
ATOM	1459	O	LEU	A	564	34.350	8.918	14.034	1.00	4.33	O
ATOM	1460	N	SER	A	565	34.677	9.272	11.849	1.00	4.86	N
ATOM	1461	CA	SER	A	565	35.281	10.573	12.036	1.00	5.62	C
ATOM	1462	CB	SER	A	565	35.653	11.162	10.720	1.00	6.03	C
ATOM	1463	OG	SER	A	565	36.397	10.281	9.913	1.00	9.07	O
ATOM	1464	C	SER	A	565	34.368	11.553	12.711	1.00	6.16	C
ATOM	1465	O	SER	A	565	34.856	12.519	13.301	1.00	7.64	O
ATOM	1466	N	ASP	A	566	33.058	11.357	12.600	1.00	5.01	N
ATOM	1467	CA	ASP	A	566	32.118	12.194	13.356	1.00	4.61	C
ATOM	1468	CB	ASP	A	566	30.751	12.235	12.667	1.00	4.01	C
ATOM	1469	CG	ASP	A	566	30.043	10.859	12.633	1.00	7.60	C
ATOM	1470	OD1	ASP	A	566	30.719	9.768	12.582	1.00	12.23	O
ATOM	1471	OD2	ASP	A	566	28.798	10.766	12.592	1.00	6.42	O
ATOM	1472	C	ASP	A	566	31.929	11.762	14.835	1.00	4.59	C
ATOM	1473	O	ASP	A	566	31.067	12.257	15.518	1.00	6.37	O
ATOM	1474	N	SER	A	567	32.752	10.892	15.365	1.00	3.80	N
ATOM	1475	CA	SER	A	567	32.472	10.379	16.678	1.00	4.60	C
ATOM	1476	CB	SER	A	567	32.849	8.890	16.709	1.00	4.41	C

ATOM	1477	OG	SER A 567	32.554	8.341	17.982	1.00	5.48	O
ATOM	1478	C	SER A 567	33.115	11.092	17.875	1.00	4.42	C
ATOM	1479	O	SER A 567	34.332	11.220	17.963	1.00	4.31	O
ATOM	1480	N	PRO A 568	32.300	11.423	18.867	1.00	4.48	N
ATOM	1481	CA	PRO A 568	32.786	12.087	20.083	1.00	4.54	C
ATOM	1482	CB	PRO A 568	31.550	12.119	20.963	1.00	4.15	C
ATOM	1483	CG	PRO A 568	30.425	12.026	20.031	1.00	4.02	C
ATOM	1484	CD	PRO A 568	30.859	11.141	18.927	1.00	3.92	C
ATOM	1485	C	PRO A 568	33.922	11.300	20.746	1.00	4.80	C
ATOM	1486	O	PRO A 568	34.778	11.860	21.382	1.00	5.03	O
ATOM	1487	N	LEU A 569	33.962	9.997	20.550	1.00	5.56	N
ATOM	1488	CA	LEU A 569	35.065	9.185	21.063	1.00	5.83	C
ATOM	1489	CB	LEU A 569	34.953	7.839	20.393	1.00	5.39	C
ATOM	1490	CG	LEU A 569	35.662	6.643	21.012	1.00	8.02	C
ATOM	1491	CD1	LEU A 569	36.514	5.968	20.035	1.00	7.12	C
ATOM	1492	CD2	LEU A 569	36.445	7.041	22.339	1.00	9.13	C
ATOM	1493	C	LEU A 569	36.523	9.780	20.895	1.00	6.51	C
ATOM	1494	O	LEU A 569	37.338	9.766	21.816	1.00	7.17	O
ATOM	1495	N	PHE A 570	36.860	10.317	19.739	1.00	6.86	N
ATOM	1496	CA	PHE A 570	38.216	10.808	19.528	1.00	7.23	C
ATOM	1497	CB	PHE A 570	38.501	11.136	18.035	1.00	5.23	C
ATOM	1498	CG	PHE A 570	38.424	9.923	17.163	1.00	6.73	C
ATOM	1499	CD1	PHE A 570	39.368	8.914	17.301	1.00	7.09	C
ATOM	1500	CE1	PHE A 570	39.276	7.757	16.572	1.00	7.82	C
ATOM	1501	CZ	PHE A 570	38.233	7.573	15.679	1.00	7.51	C
ATOM	1502	CE2	PHE A 570	37.301	8.556	15.528	1.00	6.38	C
ATOM	1503	CD2	PHE A 570	37.377	9.719	16.292	1.00	5.05	C
ATOM	1504	C	PHE A 570	38.524	11.975	20.418	1.00	9.18	C
ATOM	1505	O	PHE A 570	39.718	12.193	20.765	1.00	10.62	O
ATOM	1506	N	ASP A 571	37.494	12.747	20.782	1.00	10.38	N
ATOM	1507	CA	ASP A 571	37.678	13.891	21.705	1.00	12.23	C
ATOM	1508	CB	ASP A 571	36.503	14.908	21.636	1.00	12.92	C
ATOM	1509	CG	ASP A 571	36.747	16.079	20.592	1.00	19.58	C
ATOM	1510	OD1	ASP A 571	35.738	16.784	20.221	1.00	22.58	O
ATOM	1511	OD2	ASP A 571	37.892	16.388	20.102	1.00	24.68	O
ATOM	1512	C	ASP A 571	37.838	13.320	23.139	1.00	11.69	C
ATOM	1513	O	ASP A 571	38.703	13.723	23.898	1.00	9.05	O
ATOM	1514	N	LEU A 572	37.023	12.322	23.447	1.00	12.36	N

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ATOM   1515  CA  LEU A 572      37.111  11.657  24.705  1.00 14.85           C
ATOM   1516  CB  LEU A 572      36.028  10.621  24.800  1.00 16.18           C
ATOM   1517  CG  LEU A 572      35.809  10.127  26.233  1.00 21.52           C
ATOM   1518  CD1 LEU A 572      35.722  11.348  27.185  1.00 21.46           C
ATOM   1519  CD2 LEU A 572      34.536   9.247  26.291  1.00 23.88           C
ATOM   1520  C   LEU A 572      38.461  10.963  24.850  1.00 15.08           O
ATOM   1521  O   LEU A 572      38.945  10.761  25.954  1.00 15.22           N
ATOM   1522  N   ILE A 573      39.068  10.567  23.745  1.00 15.07           C
ATOM   1523  CA  ILE A 573      40.376   9.968  23.850  1.00 15.55           C
ATOM   1524  CB  ILE A 573      40.645   9.090  22.628  1.00 14.55           C
ATOM   1525  CG1 ILE A 573      39.959   7.746  22.767  1.00 12.31           C
ATOM   1526  CD1 ILE A 573      39.857   6.981  21.393  1.00  6.14           C
ATOM   1527  CG2 ILE A 573      42.098   8.825  22.425  1.00 12.90           C
ATOM   1528  C   ILE A 573      41.435  11.088  23.983  1.00 17.30           C
ATOM   1529  O   ILE A 573      42.414  10.949  24.685  1.00 18.35           O
ATOM   1530  N   LYS A 574      41.261  12.192  23.290  1.00 17.39           N
ATOM   1531  CA  LYS A 574      42.272  13.190  23.373  1.00 18.15           C
ATOM   1532  CB  LYS A 574      42.087  14.242  22.296  1.00 16.97           C
ATOM   1533  CG  LYS A 574      43.280  15.079  22.098  1.00 15.24           C
ATOM   1534  CD  LYS A 574      43.072  16.241  21.114  1.00 15.89           C
ATOM   1535  CE  LYS A 574      44.287  17.213  21.136  1.00 14.11           C
ATOM   1536  NZ  LYS A 574      44.345  18.197  20.020  1.00  9.92           N
ATOM   1537  C   LYS A 574      42.251  13.802  24.760  1.00 20.35           C
ATOM   1538  O   LYS A 574      43.302  13.946  25.401  1.00 20.46           O
ATOM   1539  N   GLN A 575      41.059  14.149  25.224  1.00 22.46           N
ATOM   1540  CA  GLN A 575      40.876  14.743  26.532  1.00 24.95           C
ATOM   1541  CB  GLN A 575      39.394  14.789  26.845  1.00 25.51           C
ATOM   1542  CG  GLN A 575      39.020  15.353  28.210  1.00 31.74           C
ATOM   1543  CD  GLN A 575      37.544  15.802  28.301  1.00 36.07           C
ATOM   1544  OE1 GLN A 575      36.639  14.979  28.181  1.00 37.48           O
ATOM   1545  NE2 GLN A 575      37.315  17.110  28.535  1.00 37.16           N
ATOM   1546  C   GLN A 575      41.569  13.876  27.560  1.00 26.44           C
ATOM   1547  O   GLN A 575      42.042  14.356  28.570  1.00 26.79           O
ATOM   1548  N   SER A 576      41.660  12.579  27.291  1.00 28.20           N
ATOM   1549  CA  SER A 576      42.287  11.655  28.238  1.00 28.79           C
ATOM   1550  CB  SER A 576      41.622  10.312  28.144  1.00 28.17           C
ATOM   1551  OG  SER A 576      42.636   9.371  27.953  1.00 27.25           O
ATOM   1552  C   SER A 576      43.775  11.452  28.024  1.00 29.76           C
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ATOM   1553  O   SER A 576      44.506  11.186  28.946  1.00 29.92           O
ATOM   1554  N   LYS A 577      44.210  11.566  26.785  1.00 31.31           N
ATOM   1555  CA  LYS A 577      45.610  11.424  26.438  1.00 32.44           C
ATOM   1556  CB  LYS A 577      45.756  11.456  24.924  1.00 32.43           C
ATOM   1557  CG  LYS A 577      46.759  10.514  24.390  1.00 31.18           C
ATOM   1558  CD  LYS A 577      46.252   9.097  24.601  1.00 28.82           C
ATOM   1559  CE  LYS A 577      47.095   8.118  23.806  1.00 29.90           C
ATOM   1560  NZ  LYS A 577      46.930   6.691  24.174  1.00 25.38           N
ATOM   1561  C   LYS A 577      46.462  12.556  27.028  1.00 33.67           C
ATOM   1562  O   LYS A 577      47.676  12.565  26.875  1.00 33.03           O
ATOM   1563  N   ASP A 578      45.820  13.534  27.663  1.00 35.46           N
ATOM   1564  CA  ASP A 578      46.552  14.659  28.239  1.00 36.42           C
ATOM   1565  CB  ASP A 578      45.949  16.006  27.817  1.00 36.95           C
ATOM   1566  CG  ASP A 578      46.096  16.280  26.331  1.00 38.84           C
ATOM   1567  OD1 ASP A 578      47.060  15.800  25.685  1.00 41.17           O
ATOM   1568  OD2 ASP A 578      45.279  16.976  25.708  1.00 42.67           O
ATOM   1569  C   ASP A 578      46.556  14.554  29.751  1.00 36.86           C
ATOM   1573  N   SER B 644      36.636   9.547  33.813  1.00 13.34           N
ATOM   1574  CA  SER B 644      35.896   9.256  32.537  1.00 13.52           C
ATOM   1575  CB  SER B 644      36.738   9.648  31.317  1.00 14.13           C
ATOM   1576  OG  SER B 644      35.927   9.799  30.153  1.00 17.99           O
ATOM   1577  C   SER B 644      35.367   7.811  32.424  1.00 12.17           C
ATOM   1578  O   SER B 644      35.897   6.982  31.701  1.00 12.64           O
ATOM   1579  N   THR B 645      34.293   7.546  33.159  1.00 10.72           N
ATOM   1580  CA  THR B 645      33.630   6.265  33.190  1.00  8.91           C
ATOM   1581  CB  THR B 645      32.330   6.374  34.033  1.00  9.09           C
ATOM   1582  OG1 THR B 645      32.625   6.834  35.352  1.00  8.17           O
ATOM   1583  CG2 THR B 645      31.728   4.968  34.256  1.00  9.39           C
ATOM   1584  C   THR B 645      33.274   5.785  31.770  1.00  7.52           C
ATOM   1585  O   THR B 645      33.531   4.625  31.379  1.00  5.65           O
ATOM   1586  N   SER B 646      32.676   6.694  31.028  1.00  6.11           N
ATOM   1587  CA  SER B 646      32.310   6.460  29.633  1.00  6.99           C
ATOM   1588  CB  SER B 646      31.925   7.758  28.930  1.00  7.51           C
ATOM   1589  OG  SER B 646      32.996   8.717  29.121  1.00 12.87           O
ATOM   1590  C   SER B 646      33.444   5.841  28.850  1.00  4.97           C
ATOM   1591  O   SER B 646      33.254   4.809  28.273  1.00  3.36           O
ATOM   1592  N   LEU B 647      34.606   6.477  28.859  1.00  4.50           N
ATOM   1593  CA  LEU B 647      35.742   5.969  28.104  1.00  6.01           C
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ATOM   1594  CB  LEU B 647      36.846   6.981  28.058  1.00  6.07           C
ATOM   1595  CG  LEU B 647      38.046   6.586  27.214  1.00  5.64           C
ATOM   1596  CD1 LEU B 647      37.711   6.400  25.743  1.00  2.00           C
ATOM   1597  CD2 LEU B 647      39.120   7.685  27.433  1.00  3.27           C
ATOM   1598  C   LEU B 647      36.327   4.653  28.634  1.00  7.62           C
ATOM   1599  O   LEU B 647      36.803   3.822  27.846  1.00  7.75           O
ATOM   1600  N   SER B 648      36.335   4.459  29.958  1.00  7.31           N
ATOM   1601  CA  SER B 648      36.813   3.191  30.458  1.00  7.43           C
ATOM   1602  CB  SER B 648      37.232   3.312  31.940  1.00  8.38           C
ATOM   1603  OG  SER B 648      36.099   3.311  32.774  1.00 12.14           O
ATOM   1604  C   SER B 648      35.783   2.054  30.271  1.00  6.33           C
ATOM   1605  O   SER B 648      36.135   0.897  30.113  1.00  6.45           O
ATOM   1606  N   LEU B 649      34.499   2.359  30.278  1.00  5.67           N
ATOM   1607  CA  LEU B 649      33.485   1.304  30.061  1.00  4.38           C
ATOM   1608  CB  LEU B 649      32.075   1.863  30.294  1.00  3.95           C
ATOM   1609  CG  LEU B 649      30.936   0.916  30.609  1.00  3.72           C
ATOM   1610  CD1 LEU B 649      30.121   0.646  29.371  1.00  8.06           C
ATOM   1611  CD2 LEU B 649      31.444  -0.408  31.175  1.00  2.00           C
ATOM   1612  C   LEU B 649      33.590   0.812  28.646  1.00  4.70           C
ATOM   1613  O   LEU B 649      33.553  -0.418  28.356  1.00  6.51           O
ATOM   1614  N   PHE B 650      33.796   1.774  27.755  1.00  3.18           N
ATOM   1615  CA  PHE B 650      33.888   1.510  26.366  1.00  2.00           C
ATOM   1616  CB  PHE B 650      33.940   2.828  25.556  1.00  2.00           C
ATOM   1617  CG  PHE B 650      33.947   2.604  24.106  1.00  2.00           C
ATOM   1618  CD1 PHE B 650      32.763   2.357  23.427  1.00  2.00           C
ATOM   1619  CE1 PHE B 650      32.792   2.111  22.035  1.00  2.00           C
ATOM   1620  CZ  PHE B 650      33.988   2.062  21.329  1.00  2.00           C
ATOM   1621  CE2 PHE B 650      35.175   2.284  21.992  1.00  2.00           C
ATOM   1622  CD2 PHE B 650      35.163   2.543  23.394  1.00  2.00           C
ATOM   1623  C   PHE B 650      35.103   0.619  26.111  1.00  2.00           C
ATOM   1624  O   PHE B 650      34.994  -0.415  25.474  1.00  2.37           O
ATOM   1625  N   TYR B 651      36.266   1.031  26.556  1.00  2.00           N
ATOM   1626  CA  TYR B 651      37.452   0.270  26.268  1.00  3.35           C
ATOM   1627  CB  TYR B 651      38.731   0.988  26.767  1.00  3.37           C
ATOM   1628  CG  TYR B 651      39.419   1.741  25.662  1.00  4.03           C
ATOM   1629  CD1 TYR B 651      40.287   1.076  24.801  1.00  5.03           C
ATOM   1630  CE1 TYR B 651      40.882   1.737  23.744  1.00  7.04           C
ATOM   1631  CZ  TYR B 651      40.633   3.096  23.506  1.00  3.43           C
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ATOM   1632  OH  TYR B 651      41.249   3.679  22.433  1.00  3.35           O
ATOM   1633  CE2 TYR B 651      39.780   3.780  24.300  1.00  2.37           C
ATOM   1634  CD2 TYR B 651      39.147   3.087  25.408  1.00  2.56           C
ATOM   1635  C   TYR B 651      37.335  -1.135  26.856  1.00  4.60           C
ATOM   1636  O   TYR B 651      37.557  -2.180  26.169  1.00  3.86           O
ATOM   1637  N   LYS B 652      36.925  -1.165  28.109  1.00  5.25           N
ATOM   1638  CA  LYS B 652      36.770  -2.429  28.776  1.00  7.08           C
ATOM   1639  CB  LYS B 652      36.116  -2.190  30.135  1.00  9.45           C
ATOM   1640  CG  LYS B 652      36.103  -3.327  31.124  1.00  9.85           C
ATOM   1641  CD  LYS B 652      35.793  -2.711  32.483  1.00  8.46           C
ATOM   1642  CE  LYS B 652      34.602  -3.426  33.172  1.00 11.02           C
ATOM   1643  NZ  LYS B 652      34.713  -4.916  33.235  1.00 10.84           N
ATOM   1644  C   LYS B 652      35.971  -3.380  27.910  1.00  6.24           C
ATOM   1645  O   LYS B 652      36.417  -4.472  27.586  1.00  6.42           O
ATOM   1646  N   LYS B 653      34.803  -2.965  27.484  1.00  6.01           N
ATOM   1647  CA  LYS B 653      34.039  -3.842  26.566  1.00  5.79           C
ATOM   1648  CB  LYS B 653      32.592  -3.355  26.388  1.00  6.75           C
ATOM   1649  CG  LYS B 653      31.683  -3.588  27.623  1.00  6.98           C
ATOM   1650  CD  LYS B 653      30.444  -2.803  27.531  1.00  9.41           C
ATOM   1651  CE  LYS B 653      29.457  -3.240  28.518  1.00  9.56           C
ATOM   1652  NZ  LYS B 653      29.069  -4.552  28.071  1.00 16.84           N
ATOM   1653  C   LYS B 653      34.665  -4.068  25.177  1.00  5.15           C
ATOM   1654  O   LYS B 653      34.680  -5.204  24.665  1.00  5.64           O
ATOM   1655  N   VAL B 654      35.172  -3.033  24.528  1.00  3.96           N
ATOM   1656  CA  VAL B 654      35.796  -3.311  23.240  1.00  4.21           C
ATOM   1657  CB  VAL B 654      36.340  -2.025  22.582  1.00  3.09           C
ATOM   1658  CG1 VAL B 654      37.138  -2.320  21.425  1.00  4.47           C
ATOM   1659  CG2 VAL B 654      35.261  -1.175  22.068  1.00  3.53           C
ATOM   1660  C   VAL B 654      36.923  -4.399  23.425  1.00  5.38           C
ATOM   1661  O   VAL B 654      37.162  -5.194  22.517  1.00  5.50           O
ATOM   1662  N   TYR B 655      37.606  -4.433  24.579  1.00  4.72           N
ATOM   1663  CA  TYR B 655      38.644  -5.454  24.769  1.00  6.51           C
ATOM   1664  CB  TYR B 655      39.505  -5.204  26.019  1.00  6.11           C
ATOM   1665  CG  TYR B 655      40.456  -4.016  25.925  1.00  9.57           C
ATOM   1666  CD1 TYR B 655      41.074  -3.656  24.712  1.00 10.61           C
ATOM   1667  CE1 TYR B 655      41.943  -2.567  24.654  1.00 12.73           C
ATOM   1668  CZ  TYR B 655      42.195  -1.858  25.839  1.00 13.88           C
ATOM   1669  OH  TYR B 655      43.039  -0.758  25.867  1.00 17.21           O
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ATOM	1670	CE2	TYR	B	655	41.577	-2.206	27.021	1.00	8.69	C
ATOM	1671	CD2	TYR	B	655	40.725	-3.241	27.055	1.00	9.00	C
ATOM	1672	C	TYR	B	655	38.074	-6.888	24.825	1.00	6.04	C
ATOM	1673	O	TYR	B	655	38.605	-7.806	24.221	1.00	6.92	O
ATOM	1674	N	ARG	B	656	36.985	-7.059	25.528	1.00	5.36	N
ATOM	1675	CA	ARG	B	656	36.402	-8.358	25.720	1.00	6.12	C
ATOM	1676	CB	ARG	B	656	35.157	-8.238	26.641	1.00	5.83	C
ATOM	1677	CG	ARG	B	656	34.955	-9.400	27.555	1.00	9.85	C
ATOM	1678	CD	ARG	B	656	33.527	-9.895	27.730	1.00	14.72	C
ATOM	1679	NE	ARG	B	656	33.278	-10.215	29.135	1.00	19.73	N
ATOM	1680	CZ	ARG	B	656	32.174	-10.816	29.568	1.00	23.51	C
ATOM	1681	NH1	ARG	B	656	31.217	-11.188	28.707	1.00	26.59	N
ATOM	1682	NH2	ARG	B	656	32.021	-11.056	30.851	1.00	19.55	N
ATOM	1683	C	ARG	B	656	36.008	-8.885	24.362	1.00	5.96	C
ATOM	1684	O	ARG	B	656	36.360	-9.999	24.006	1.00	5.87	O
ATOM	1685	N	LEU	B	657	35.272	-8.056	23.612	1.00	6.37	N
ATOM	1686	CA	LEU	B	657	34.794	-8.416	22.293	1.00	6.12	C
ATOM	1687	CB	LEU	B	657	34.122	-7.226	21.632	1.00	5.46	C
ATOM	1688	CG	LEU	B	657	32.951	-7.388	20.640	1.00	7.16	C
ATOM	1689	CD1	LEU	B	657	33.118	-6.470	19.460	1.00	2.00	C
ATOM	1690	CD2	LEU	B	657	32.700	-8.824	20.156	1.00	5.57	C
ATOM	1691	C	LEU	B	657	36.009	-8.820	21.465	1.00	6.67	C
ATOM	1692	O	LEU	B	657	36.065	-9.905	20.924	1.00	6.08	O
ATOM	1693	N	ALA	B	658	37.004	-7.943	21.405	1.00	7.27	N
ATOM	1694	CA	ALA	B	658	38.156	-8.168	20.556	1.00	7.68	C
ATOM	1695	CB	ALA	B	658	39.093	-7.045	20.658	1.00	9.00	C
ATOM	1696	C	ALA	B	658	38.893	-9.422	20.884	1.00	8.43	C
ATOM	1697	O	ALA	B	658	39.271	-10.196	19.981	1.00	8.28	O
ATOM	1698	N	TYR	B	659	39.143	-9.615	22.174	1.00	8.68	N
ATOM	1699	CA	TYR	B	659	39.850	-10.806	22.595	1.00	8.59	C
ATOM	1700	CB	TYR	B	659	40.177	-10.769	24.087	1.00	8.82	C
ATOM	1701	CG	TYR	B	659	40.775	-12.110	24.491	1.00	11.54	C
ATOM	1702	CD1	TYR	B	659	42.087	-12.435	24.133	1.00	7.96	C
ATOM	1703	CE1	TYR	B	659	42.608	-13.629	24.463	1.00	12.41	C
ATOM	1704	CZ	TYR	B	659	41.822	-14.579	25.146	1.00	14.10	C
ATOM	1705	OH	TYR	B	659	42.353	-15.803	25.433	1.00	10.91	O
ATOM	1706	CE2	TYR	B	659	40.511	-14.296	25.495	1.00	12.41	C
ATOM	1707	CD2	TYR	B	659	39.996	-13.070	25.164	1.00	11.29	C

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ATOM   1708  C   TYR B 659      39.053 -12.090  22.229  1.00  8.10           C
ATOM   1709  O   TYR B 659      39.591 -13.017  21.663  1.00  7.91           O
ATOM   1710  N   LEU B 660      37.773 -12.143  22.548  1.00  8.11           N
ATOM   1711  CA  LEU B 660      36.976 -13.330  22.205  1.00  8.99           C
ATOM   1712  CB  LEU B 660      35.494 -13.149  22.601  1.00  8.89           C
ATOM   1713  CG  LEU B 660      35.270 -13.204  24.110  1.00  9.33           C
ATOM   1714  CD1 LEU B 660      33.943 -12.684  24.547  1.00  9.61           C
ATOM   1715  CD2 LEU B 660      35.439 -14.643  24.553  1.00  9.83           C
ATOM   1716  C   LEU B 660      37.054 -13.675  20.721  1.00  9.42           O
ATOM   1717  O   LEU B 660      37.057 -14.831  20.349  1.00  9.34           N
ATOM   1718  N   ARG B 661      37.054 -12.663  19.860  1.00  9.71           C
ATOM   1719  CA  ARG B 661      37.050 -12.968  18.462  1.00 10.45           C
ATOM   1720  CB  ARG B 661      36.608 -11.793  17.653  1.00  8.53           C
ATOM   1721  CG  ARG B 661      35.229 -11.304  17.915  1.00  7.97           C
ATOM   1722  CD  ARG B 661      34.886 -10.027  17.178  1.00  3.76           C
ATOM   1723  NE  ARG B 661      33.472  -9.762  16.983  1.00  2.70           N
ATOM   1724  CZ  ARG B 661      32.973  -8.629  16.467  1.00  3.60           C
ATOM   1725  NH1 ARG B 661      33.784  -7.652  16.053  1.00  3.87           N
ATOM   1726  NH2 ARG B 661      31.652  -8.468  16.330  1.00  2.00           N
ATOM   1727  C   ARG B 661      38.478 -13.448  18.096  1.00 12.78           C
ATOM   1728  O   ARG B 661      38.625 -14.338  17.273  1.00 13.90           O
ATOM   1729  N   LEU B 662      39.508 -12.879  18.735  1.00 13.10           N
ATOM   1730  CA  LEU B 662      40.902 -13.230  18.462  1.00 13.72           C
ATOM   1731  CB  LEU B 662      41.803 -12.308  19.265  1.00 13.06           C
ATOM   1732  CG  LEU B 662      43.286 -12.110  18.918  1.00 14.40           C
ATOM   1733  CD1 LEU B 662      44.132 -12.325  20.086  1.00  9.20           C
ATOM   1734  CD2 LEU B 662      43.829 -12.854  17.630  1.00 15.62           C
ATOM   1735  C   LEU B 662      41.198 -14.658  18.904  1.00 15.28           C
ATOM   1736  O   LEU B 662      41.900 -15.448  18.206  1.00 15.63           O
ATOM   1737  N   ASN B 663      40.656 -14.980  20.082  1.00 15.58           N
ATOM   1738  CA  ASN B 663      40.829 -16.268  20.666  1.00 15.36           C
ATOM   1739  CB  ASN B 663      40.287 -16.291  22.090  1.00 15.75           C
ATOM   1740  CG  ASN B 663      40.059 -17.727  22.606  1.00 16.02           C
ATOM   1741  OD1 ASN B 663      38.985 -18.274  22.388  1.00 16.31           O
ATOM   1742  ND2 ASN B 663      41.057 -18.320  23.284  1.00  9.15           N
ATOM   1743  C   ASN B 663      40.143 -17.296  19.840  1.00 15.24           C
ATOM   1744  O   ASN B 663      40.592 -18.403  19.771  1.00 15.75           O
ATOM   1745  N   THR B 664      39.030 -16.930  19.225  1.00 15.92           N
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ATOM   1746  CA  THR B 664      38.274 -17.868  18.396  1.00 15.65           C
ATOM   1747  CB  THR B 664      36.934 -17.267  17.986  1.00 16.03           C
ATOM   1748  OG1 THR B 664      36.179 -16.882  19.145  1.00 18.60           O
ATOM   1749  CG2 THR B 664      36.076 -18.315  17.271  1.00 12.83           C
ATOM   1750  C   THR B 664      39.059 -18.201  17.126  1.00 15.89           C
ATOM   1751  O   THR B 664      39.095 -19.335  16.740  1.00 15.40           O
ATOM   1752  N   LEU B 665      39.661 -17.208  16.472  1.00 16.10           N
ATOM   1753  CA  LEU B 665      40.453 -17.463  15.290  1.00 17.99           C
ATOM   1754  CB  LEU B 665      40.700 -16.171  14.515  1.00 18.03           C
ATOM   1755  CG  LEU B 665      39.504 -15.473  13.840  1.00 17.81           C
ATOM   1756  CD1 LEU B 665      39.932 -14.082  13.322  1.00 14.11           C
ATOM   1757  CD2 LEU B 665      38.978 -16.273  12.715  1.00 15.62           C
ATOM   1758  C   LEU B 665      41.816 -18.142  15.599  1.00 18.90           C
ATOM   1759  O   LEU B 665      42.290 -18.978  14.843  1.00 18.38           O
ATOM   1760  N   CYS B 666      42.452 -17.769  16.702  1.00 19.38           N
ATOM   1761  CA  CYS B 666      43.727 -18.381  17.036  1.00 19.52           C
ATOM   1762  CB  CYS B 666      44.435 -17.649  18.192  1.00 20.43           C
ATOM   1763  SG  CYS B 666      45.104 -16.057  17.678  1.00 19.13           S
ATOM   1764  C   CYS B 666      43.614 -19.808  17.430  1.00 19.42           C
ATOM   1765  O   CYS B 666      44.601 -20.549  17.260  1.00 19.57           O
ATOM   1766  N   GLU B 667      42.463 -20.191  18.009  1.00 18.97           N
ATOM   1767  CA  GLU B 667      42.273 -21.576  18.478  1.00 18.84           C
ATOM   1768  CB  GLU B 667      41.170 -21.680  19.536  1.00 18.36           C
ATOM   1769  CG  GLU B 667      40.892 -23.085  20.048  1.00 17.77           C
ATOM   1770  CD  GLU B 667      40.404 -23.151  21.526  1.00 18.28           C
ATOM   1771  OE1 GLU B 667      39.851 -24.235  21.937  1.00 12.51           O
ATOM   1772  OE2 GLU B 667      40.586 -22.126  22.277  1.00 16.34           O
ATOM   1773  C   GLU B 667      42.019 -22.508  17.291  1.00 19.46           C
ATOM   1774  O   GLU B 667      42.257 -23.691  17.387  1.00 20.81           O
ATOM   1775  N   ARG B 668      41.558 -21.979  16.166  1.00 18.39           N
ATOM   1776  CA  ARG B 668      41.330 -22.817  15.012  1.00 18.41           C
ATOM   1777  CB  ARG B 668      40.005 -22.454  14.376  1.00 19.07           C
ATOM   1778  CG  ARG B 668      38.775 -22.369  15.341  1.00 20.80           C
ATOM   1779  CD  ARG B 668      37.477 -21.891  14.616  1.00 19.53           C
ATOM   1780  NE  ARG B 668      36.292 -21.858  15.484  1.00 23.37           N
ATOM   1781  CZ  ARG B 668      35.058 -21.419  15.127  1.00 22.67           C
ATOM   1782  NH1 ARG B 668      34.778 -20.972  13.896  1.00 20.39           N
ATOM   1783  NH2 ARG B 668      34.094 -21.407  16.035  1.00 20.67           N
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ATOM   1784  C   ARG B 668      42.450 -22.719  13.950  1.00 18.34           C
ATOM   1785  O   ARG B 668      42.651 -23.613  13.122  1.00 17.26           O
ATOM   1786  N   LEU B 669      43.206 -21.630  13.988  1.00 18.42           N
ATOM   1787  CA  LEU B 669      44.255 -21.413  13.001  1.00 18.63           C
ATOM   1788  CB  LEU B 669      44.105 -19.999  12.412  1.00 19.29           C
ATOM   1789  CG  LEU B 669      43.433 -19.874  11.029  1.00 20.70           C
ATOM   1790  CD1 LEU B 669      42.191 -20.771  10.861  1.00 18.65           C
ATOM   1791  CD2 LEU B 669      43.167 -18.385  10.606  1.00 15.39           C
ATOM   1792  C   LEU B 669      45.677 -21.649  13.553  1.00 18.31           C
ATOM   1793  O   LEU B 669      46.559 -22.131  12.850  1.00 17.46           O
ATOM   1794  N   LEU B 670      45.892 -21.320  14.819  1.00 17.97           N
ATOM   1795  CA  LEU B 670      47.206 -21.450  15.382  1.00 18.50           C
ATOM   1796  CB  LEU B 670      47.699 -20.070  15.762  1.00 18.75           C
ATOM   1797  CG  LEU B 670      47.828 -19.118  14.568  1.00 17.36           C
ATOM   1798  CD1 LEU B 670      48.413 -17.828  15.007  1.00 15.48           C
ATOM   1799  CD2 LEU B 670      48.698 -19.778  13.477  1.00 14.62           C
ATOM   1800  C   LEU B 670      47.340 -22.401  16.552  1.00 19.33           C
ATOM   1801  O   LEU B 670      48.121 -22.162  17.448  1.00 19.41           O
ATOM   1802  N   SER B 671      46.646 -23.529  16.514  1.00 21.39           N
ATOM   1803  CA  SER B 671      46.704 -24.470  17.632  1.00 23.09           C
ATOM   1804  CB  SER B 671      45.665 -25.575  17.484  1.00 22.45           C
ATOM   1805  OG  SER B 671      45.803 -26.222  16.227  1.00 23.79           O
ATOM   1806  C   SER B 671      48.081 -25.084  17.765  1.00 24.29           C
ATOM   1807  O   SER B 671      48.467 -25.474  18.858  1.00 24.66           O
ATOM   1808  N   GLU B 672      48.806 -25.180  16.644  1.00 25.50           N
ATOM   1809  CA  GLU B 672      50.152 -25.749  16.637  1.00 25.94           C
ATOM   1810  CB  GLU B 672      50.715 -25.898  15.221  1.00 27.18           C
ATOM   1811  CG  GLU B 672      49.983 -26.842  14.267  1.00 31.37           C
ATOM   1812  CD  GLU B 672      50.420 -26.667  12.787  1.00 36.21           C
ATOM   1813  OE1 GLU B 672      50.113 -25.634  12.135  1.00 34.47           O
ATOM   1814  OE2 GLU B 672      51.058 -27.605  12.247  1.00 40.18           O
ATOM   1815  C   GLU B 672      51.097 -24.868  17.431  1.00 25.14           C
ATOM   1816  O   GLU B 672      52.048 -25.379  18.006  1.00 25.38           O
ATOM   1817  N   HIS B 673      50.867 -23.548  17.439  1.00 24.39           N
ATOM   1818  CA  HIS B 673      51.727 -22.613  18.226  1.00 23.25           C
ATOM   1819  CB  HIS B 673      52.507 -21.670  17.308  1.00 22.74           C
ATOM   1820  CG  HIS B 673      52.982 -22.304  16.035  1.00 24.74           C
ATOM   1821  ND1 HIS B 673      52.234 -22.309  14.874  1.00 23.69           N
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ATOM   1822  CE1 HIS B 673      52.909 -22.931  13.920  1.00 23.68           C
ATOM   1823  NE2 HIS B 673      54.075 -23.316  14.413  1.00 23.92           N
ATOM   1824  CD2 HIS B 673      54.142 -22.947  15.737  1.00 25.13           C
ATOM   1825  C   HIS B 673      50.904 -21.811  19.255  1.00 21.86           C
ATOM   1826  O   HIS B 673      50.723 -20.598  19.131  1.00 21.72           O
ATOM   1827  N   PRO B 674      50.422 -22.506  20.274  1.00 20.75           N
ATOM   1828  CA  PRO B 674      49.579 -21.913  21.309  1.00 19.67           C
ATOM   1829  CB  PRO B 674      49.540 -23.021  22.379  1.00 19.92           C
ATOM   1830  CG  PRO B 674      49.687 -24.247  21.623  1.00 19.13           C
ATOM   1831  CD  PRO B 674      50.691 -23.934  20.547  1.00 20.60           C
ATOM   1832  C   PRO B 674      50.126 -20.630  21.901  1.00 18.69           O
ATOM   1833  O   PRO B 674      49.369 -19.848  22.443  1.00 18.47           O
ATOM   1834  N   GLU B 675      51.420 -20.396  21.773  1.00 18.13           N
ATOM   1835  CA  GLU B 675      51.998 -19.194  22.326  1.00 18.19           C
ATOM   1836  CB  GLU B 675      53.517 -19.319  22.414  1.00 18.97           C
ATOM   1837  CG  GLU B 675      54.274 -19.156  21.088  1.00 19.76           C
ATOM   1838  CD  GLU B 675      54.239 -20.376  20.186  1.00 18.67           O
ATOM   1839  OE1 GLU B 675      53.642 -21.410  20.560  1.00 16.34           O
ATOM   1840  OE2 GLU B 675      54.824 -20.283  19.085  1.00 18.78           O
ATOM   1841  C   GLU B 675      51.657 -17.940  21.548  1.00 17.58           C
ATOM   1842  O   GLU B 675      51.660 -16.886  22.121  1.00 18.20           O
ATOM   1843  N   LEU B 676      51.382 -18.030  20.250  1.00 16.44           N
ATOM   1844  CA  LEU B 676      51.143 -16.803  19.469  1.00 15.70           C
ATOM   1845  CB  LEU B 676      51.006 -17.104  17.965  1.00 15.18           C
ATOM   1846  CG  LEU B 676      52.243 -17.715  17.348  1.00 13.23           C
ATOM   1847  CD1 LEU B 676      52.008 -17.973  15.866  1.00 12.22           C
ATOM   1848  CD2 LEU B 676      53.405 -16.751  17.566  1.00  8.01           C
ATOM   1849  C   LEU B 676      49.986 -15.898  19.905  1.00 14.78           C
ATOM   1850  O   LEU B 676      50.038 -14.706  19.703  1.00 14.81           O
ATOM   1851  N   GLU B 677      48.933 -16.455  20.473  1.00 14.63           N
ATOM   1852  CA  GLU B 677      47.758 -15.636  20.830  1.00 14.03           C
ATOM   1853  CB  GLU B 677      46.618 -16.503  21.396  1.00 12.86           C
ATOM   1854  CG  GLU B 677      45.378 -15.737  21.847  1.00 14.72           C
ATOM   1855  CD  GLU B 677      44.387 -16.590  22.666  1.00 17.27           C
ATOM   1856  OE1 GLU B 677      43.557 -17.338  22.098  1.00 15.74           O
ATOM   1857  OE2 GLU B 677      44.427 -16.530  23.901  1.00 16.88           O
ATOM   1858  C   GLU B 677      48.062 -14.467  21.749  1.00 13.75           C
ATOM   1859  O   GLU B 677      47.589 -13.318  21.520  1.00 14.06           O
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ATOM   1860  N   HIS B 678      48.841 -14.733  22.788  1.00 13.20           N
ATOM   1861  CA  HIS B 678      49.142 -13.689  23.765  1.00 14.08           C
ATOM   1862  CB  HIS B 678      49.775 -14.274  25.031  1.00 14.28           C
ATOM   1863  CG  HIS B 678      49.611 -13.422  26.257  1.00 16.75           C
ATOM   1864  ND1 HIS B 678      48.616 -12.466  26.386  1.00 18.50           N
ATOM   1865  CE1 HIS B 678      48.698 -11.904  27.580  1.00 17.30           C
ATOM   1866  NE2 HIS B 678      49.721 -12.439  28.220  1.00 16.02           N
ATOM   1867  CD2 HIS B 678      50.306 -13.393  27.418  1.00 15.51           C
ATOM   1868  C   HIS B 678      50.019 -12.585  23.184  1.00 13.46           C
ATOM   1869  O   HIS B 678      49.895 -11.445  23.578  1.00 13.27           O
ATOM   1870  N   ILE B 679      50.907 -12.922  22.248  1.00 13.66           N
ATOM   1871  CA  ILE B 679      51.758 -11.903  21.623  1.00 13.87           C
ATOM   1872  CB  ILE B 679      52.940 -12.548  20.884  1.00 14.37           C
ATOM   1873  CG1 ILE B 679      53.840 -13.349  21.826  1.00 15.38           C
ATOM   1874  CD1 ILE B 679      54.959 -14.175  21.105  1.00 11.31           C
ATOM   1875  CG2 ILE B 679      53.795 -11.481  20.210  1.00 16.19           C
ATOM   1876  C   ILE B 679      50.914 -11.020  20.660  1.00 13.66           C
ATOM   1877  O   ILE B 679      51.018  -9.776  20.652  1.00 12.95           O
ATOM   1878  N   ILE B 680      50.072 -11.675  19.860  1.00 12.55           N
ATOM   1879  CA  ILE B 680      49.162 -10.987  18.958  1.00 11.61           C
ATOM   1880  CB  ILE B 680      48.355 -12.008  18.110  1.00 11.65           C
ATOM   1881  CG1 ILE B 680      49.280 -12.924  17.344  1.00  9.78           C
ATOM   1882  CD1 ILE B 680      48.562 -13.950  16.468  1.00  9.87           C
ATOM   1883  CG2 ILE B 680      47.473 -11.289  17.076  1.00 12.42           C
ATOM   1884  C   ILE B 680      48.199 -10.085  19.727  1.00 11.07           C
ATOM   1885  O   ILE B 680      47.921  -8.939  19.315  1.00 10.14           O
ATOM   1886  N   TRP B 681      47.693 -10.596  20.844  1.00 10.25           N
ATOM   1887  CA  TRP B 681      46.736  -9.810  21.625  1.00  9.98           C
ATOM   1888  CB  TRP B 681      46.107 -10.594  22.784  1.00 10.30           C
ATOM   1889  CG  TRP B 681      45.516  -9.703  23.783  1.00 10.20           C
ATOM   1890  CD1 TRP B 681      45.943  -9.489  25.083  1.00  8.14           C
ATOM   1891  NE1 TRP B 681      45.123  -8.570  25.691  1.00 11.57           N
ATOM   1892  CE2 TRP B 681      44.174  -8.153  24.780  1.00 10.57           C
ATOM   1893  CD2 TRP B 681      44.396  -8.851  23.580  1.00 12.27           C
ATOM   1894  CE3 TRP B 681      43.548  -8.595  22.486  1.00 12.34           C
ATOM   1895  CZ3 TRP B 681      42.549  -7.671  22.623  1.00  8.26           C
ATOM   1896  CH2 TRP B 681      42.385  -6.984  23.815  1.00  9.93           C
ATOM   1897  CZ2 TRP B 681      43.188  -7.210  24.900  1.00  8.58           C
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ATOM	1898	C	TRP	B	681	47.427	-8.596	22.136	1.00	9.60
ATOM	1899	O	TRP	B	681	46.818	-7.521	22.282	1.00	10.07
ATOM	1900	N	THR	B	682	48.710	-8.757	22.431	1.00	9.03
ATOM	1901	CA	THR	B	682	49.523	-7.629	22.897	1.00	7.57
ATOM	1902	CB	THR	B	682	50.887	-8.117	23.316	1.00	7.89
ATOM	1903	OG1	THR	B	682	50.760	-8.912	24.499	1.00	7.20
ATOM	1904	CG2	THR	B	682	51.776	-6.939	23.723	1.00	9.26
ATOM	1905	C	THR	B	682	49.664	-6.547	21.858	1.00	5.80
ATOM	1906	O	THR	B	682	49.522	-5.428	22.192	1.00	5.05
ATOM	1907	N	LEU	B	683	50.010	-6.900	20.621	1.00	5.57
ATOM	1908	CA	LEU	B	683	50.082	-5.949	19.482	1.00	5.60
ATOM	1909	CB	LEU	B	683	50.485	-6.672	18.233	1.00	4.78
ATOM	1910	CG	LEU	B	683	51.117	-5.923	17.106	1.00	6.57
ATOM	1911	CD1	LEU	B	683	50.996	-6.590	15.661	1.00	4.62
ATOM	1912	CD2	LEU	B	683	50.646	-4.513	17.107	1.00	8.25
ATOM	1913	C	LEU	B	683	48.706	-5.331	19.208	1.00	5.57
ATOM	1914	O	LEU	B	683	48.604	-4.143	18.911	1.00	4.88
ATOM	1915	N	PHE	B	684	47.659	-6.158	19.336	1.00	6.06
ATOM	1916	CA	PHE	B	684	46.291	-5.766	19.089	1.00	6.35
ATOM	1917	CB	PHE	B	684	45.365	-6.971	19.277	1.00	6.20
ATOM	1918	CG	PHE	B	684	43.963	-6.775	18.749	1.00	5.04
ATOM	1919	CD1	PHE	B	684	43.516	-5.561	18.371	1.00	5.84
ATOM	1920	CE1	PHE	B	684	42.232	-5.363	17.912	1.00	9.04
ATOM	1921	CZ	PHE	B	684	41.368	-6.426	17.831	1.00	10.79
ATOM	1922	CE2	PHE	B	684	41.793	-7.674	18.174	1.00	10.95
ATOM	1923	CD2	PHE	B	684	43.096	-7.845	18.653	1.00	10.41
ATOM	1924	C	PHE	B	684	45.885	-4.661	20.010	1.00	6.76
ATOM	1925	O	PHE	B	684	45.351	-3.634	19.545	1.00	7.52
ATOM	1926	N	GLN	B	685	46.183	-4.856	21.293	1.00	6.72
ATOM	1927	CA	GLN	B	685	45.785	-3.957	22.379	1.00	6.81
ATOM	1928	CB	GLN	B	685	45.903	-4.668	23.756	1.00	7.65
ATOM	1929	CG	GLN	B	685	45.463	-3.884	25.038	1.00	10.43
ATOM	1930	CD	GLN	B	685	46.325	-2.667	25.299	1.00	16.01
ATOM	1931	OE1	GLN	B	685	45.818	-1.596	25.619	1.00	13.41
ATOM	1932	NE2	GLN	B	685	47.650	-2.813	25.090	1.00	17.77
ATOM	1933	C	GLN	B	685	46.597	-2.708	22.317	1.00	6.15
ATOM	1934	O	GLN	B	685	46.095	-1.608	22.604	1.00	5.65
ATOM	1935	N	HIS	B	686	47.843	-2.870	21.897	1.00	5.79

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ATOM   1936  CA  HIS B 686      48.776  -1.748  21.793  1.00  6.80           C
ATOM   1937  CB  HIS B 686      50.212  -2.230  21.429  1.00  6.29           C
ATOM   1938  CG  HIS B 686      51.124  -1.132  20.934  1.00 12.07           C
ATOM   1939  ND1 HIS B 686      51.758  -0.238  21.781  1.00 17.34           N
ATOM   1940  CE1 HIS B 686      52.481   0.616  21.068  1.00 14.84           C
ATOM   1941  NE2 HIS B 686      52.355   0.303  19.791  1.00 13.76           N
ATOM   1942  CD2 HIS B 686      51.509  -0.783  19.676  1.00 13.72           C
ATOM   1943  C   HIS B 686      48.241  -0.747  20.772  1.00  6.86           C
ATOM   1944  O   HIS B 686      48.443   0.473  20.897  1.00  5.59           O
ATOM   1945  N   THR B 687      47.531  -1.302  19.791  1.00  6.24           N
ATOM   1946  CA  THR B 687      47.058  -0.557  18.692  1.00  7.58           C
ATOM   1947  CB  THR B 687      46.784  -1.518  17.502  1.00  8.36           C
ATOM   1948  OG1 THR B 687      48.012  -2.196  17.143  1.00  6.50           O
ATOM   1949  CG2 THR B 687      46.448  -0.754  16.252  1.00  6.00           C
ATOM   1950  C   THR B 687      45.871   0.216  19.119  1.00  8.56           C
ATOM   1951  O   THR B 687      45.839   1.429  19.017  1.00 10.02           O
ATOM   1952  N   LEU B 688      44.898  -0.482  19.673  1.00  9.41           N
ATOM   1953  CA  LEU B 688      43.666   0.139  20.069  1.00  8.15           C
ATOM   1954  CB  LEU B 688      42.762  -0.907  20.687  1.00  7.39           C
ATOM   1955  CG  LEU B 688      42.153  -1.890  19.723  1.00 10.18           C
ATOM   1956  CD1 LEU B 688      41.445  -3.058  20.415  1.00  7.27           C
ATOM   1957  CD2 LEU B 688      41.142  -1.098  18.791  1.00 13.68           C
ATOM   1958  C   LEU B 688      43.962   1.272  21.036  1.00  8.20           C
ATOM   1959  O   LEU B 688      43.227   2.296  21.085  1.00  7.09           O
ATOM   1960  N   GLN B 689      45.030   1.084  21.812  1.00  8.37           N
ATOM   1961  CA  GLN B 689      45.360   2.012  22.883  1.00  9.31           C
ATOM   1962  CB  GLN B 689      45.965   1.285  24.062  1.00  9.91           C
ATOM   1963  CG  GLN B 689      46.488   2.136  25.193  1.00 11.42           C
ATOM   1964  CD  GLN B 689      47.388   1.309  26.139  1.00 17.91           C
ATOM   1965  OE1 GLN B 689      47.428   1.509  27.368  1.00 16.41           O
ATOM   1966  NE2 GLN B 689      48.116   0.373  25.548  1.00 22.03           N
ATOM   1967  C   GLN B 689      46.291   3.107  22.475  1.00 10.03           C
ATOM   1968  O   GLN B 689      46.151   4.202  22.972  1.00 10.38           O
ATOM   1969  N   ASN B 690      47.242   2.842  21.585  1.00 10.31           N
ATOM   1970  CA  ASN B 690      48.195   3.873  21.243  1.00 10.87           C
ATOM   1971  CB  ASN B 690      49.594   3.477  21.680  1.00 11.41           C
ATOM   1972  CG  ASN B 690      49.655   3.038  23.163  1.00 14.58           C
ATOM   1973  OD1 ASN B 690      49.287   3.797  24.079  1.00 12.40           O
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ATOM   1974  ND2 ASN B 690      50.129   1.806  23.395  1.00 13.56           N
ATOM   1975  C   ASN B 690      48.200   4.283  19.791  1.00 11.32           C
ATOM   1976  O   ASN B 690      48.675   5.346  19.472  1.00 12.34           O
ATOM   1977  N   GLU B 691      47.670   3.471  18.897  1.00 11.49           N
ATOM   1978  CA  GLU B 691      47.629   3.873  17.493  1.00 12.32           C
ATOM   1979  CB  GLU B 691      48.418   2.895  16.589  1.00 13.24           C
ATOM   1980  CG  GLU B 691      49.824   2.554  17.042  1.00 16.51           C
ATOM   1981  CD  GLU B 691      50.774   3.763  16.964  1.00 27.49           C
ATOM   1982  OE1 GLU B 691      50.583   4.649  16.071  1.00 28.02           O
ATOM   1983  OE2 GLU B 691      51.722   3.845  17.795  1.00 27.57           O
ATOM   1984  C   GLU B 691      46.173   3.941  17.054  1.00 11.32           C
ATOM   1985  O   GLU B 691      45.826   3.491  15.982  1.00  9.71           O
ATOM   1986  N   TYR B 692      45.346   4.520  17.925  1.00 12.17           N
ATOM   1987  CA  TYR B 692      43.892   4.662  17.749  1.00 11.54           C
ATOM   1988  CB  TYR B 692      43.246   5.296  18.968  1.00 10.36           C
ATOM   1989  CG  TYR B 692      43.781   6.634  19.276  1.00 12.35           C
ATOM   1990  CD1 TYR B 692      43.456   7.724  18.465  1.00 13.10           C
ATOM   1991  CE1 TYR B 692      43.952   8.952  18.712  1.00 12.96           C
ATOM   1992  CZ  TYR B 692      44.790   9.139  19.800  1.00 15.72           C
ATOM   1993  OH  TYR B 692      45.273  10.416  20.038  1.00 18.87           O
ATOM   1994  CE2 TYR B 692      45.130   8.076  20.641  1.00 12.33           C
ATOM   1995  CD2 TYR B 692      44.643   6.833  20.368  1.00 10.45           C
ATOM   1996  C   TYR B 692      43.456   5.375  16.481  1.00 11.74           C
ATOM   1997  O   TYR B 692      42.342   5.147  16.015  1.00 12.21           O
ATOM   1998  N   GLU B 693      44.334   6.181  15.881  1.00 11.26           N
ATOM   1999  CA  GLU B 693      43.993   6.843  14.644  1.00 10.21           C
ATOM   2000  CB  GLU B 693      45.024   7.880  14.262  1.00 10.93           C
ATOM   2001  CG  GLU B 693      44.958   9.126  15.116  1.00 12.97           C
ATOM   2002  CD  GLU B 693      43.629   9.809  15.027  1.00 16.35           C
ATOM   2003  OE1 GLU B 693      43.221  10.421  16.037  1.00 22.86           O
ATOM   2004  OE2 GLU B 693      42.974   9.751  13.961  1.00 15.98           O
ATOM   2005  C   GLU B 693      43.839   5.846  13.532  1.00  9.33           C
ATOM   2006  O   GLU B 693      43.184   6.125  12.529  1.00 10.07           O
ATOM   2007  N   LEU B 694      44.370   4.664  13.729  1.00  7.38           N
ATOM   2008  CA  LEU B 694      44.294   3.595  12.747  1.00  7.01           C
ATOM   2009  CB  LEU B 694      45.194   2.459  13.250  1.00  8.21           C
ATOM   2010  CG  LEU B 694      46.133   1.851  12.255  1.00 11.49           C
ATOM   2011  CD1 LEU B 694      46.625   2.906  11.273  1.00 11.62           C
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ATOM   2012  CD2 LEU B 694      47.261   1.293  13.091  1.00 12.03           C
ATOM   2013  C   LEU B 694      42.880   3.049  12.604  1.00  6.18           C
ATOM   2014  O   LEU B 694      42.537   2.492  11.620  1.00  4.81           O
ATOM   2015  N   MET B 695      42.079   3.163  13.645  1.00  6.55           N
ATOM   2016  CA  MET B 695      40.705   2.688  13.639  1.00  6.27           C
ATOM   2017  CB  MET B 695      40.166   2.596  15.082  1.00  7.54           C
ATOM   2018  CG  MET B 695      40.634   1.332  15.836  1.00  9.37           C
ATOM   2019  SD  MET B 695      39.938  -0.166  15.166  1.00  7.22           S
ATOM   2020  CE  MET B 695      38.323   0.077  15.495  1.00  2.00           C
ATOM   2021  C   MET B 695      39.780   3.627  12.933  1.00  5.88           C
ATOM   2022  O   MET B 695      38.662   3.212  12.616  1.00  5.11           O
ATOM   2023  N   ARG B 696      40.219   4.874  12.705  1.00  5.14           N
ATOM   2024  CA  ARG B 696      39.358   5.925  12.159  1.00  5.59           C
ATOM   2025  CB  ARG B 696      40.136   7.200  11.947  1.00  6.29           C
ATOM   2026  CG  ARG B 696      39.302   8.469  11.978  1.00  6.47           C
ATOM   2027  CD  ARG B 696      40.166   9.744  11.848  1.00  8.31           C
ATOM   2028  NE  ARG B 696      39.304  10.900  12.043  1.00 13.20           N
ATOM   2029  CZ  ARG B 696      39.133  11.587  13.185  1.00  9.34           C
ATOM   2030  NH1 ARG B 696      39.826  11.314  14.278  1.00  3.82           N
ATOM   2031  NH2 ARG B 696      38.279  12.606  13.177  1.00  9.75           N
ATOM   2032  C   ARG B 696      38.683   5.569  10.866  1.00  5.88           C
ATOM   2033  O   ARG B 696      39.321   5.442   9.835  1.00  6.24           O
ATOM   2034  N   ASP B 697      37.374   5.417  10.909  1.00  5.84           N
ATOM   2035  CA  ASP B 697      36.620   5.019   9.689  1.00  6.16           C
ATOM   2036  CB  ASP B 697      36.851   6.024   8.563  1.00  5.37           C
ATOM   2037  CG  ASP B 697      36.238   7.416   8.830  1.00  5.53           C
ATOM   2038  OD1 ASP B 697      35.077   7.547   9.309  1.00  7.21           O
ATOM   2039  OD2 ASP B 697      36.823   8.461   8.482  1.00  3.96           O
ATOM   2040  C   ASP B 697      36.989   3.586   9.232  1.00  4.52           C
ATOM   2041  O   ASP B 697      36.893   3.257   8.060  1.00  2.10           O
ATOM   2042  N   ARG B 698      37.458   2.779  10.173  1.00  2.27           N
ATOM   2043  CA  ARG B 698      37.862   1.431   9.890  1.00  3.61           C
ATOM   2044  CB  ARG B 698      39.393   1.335   9.864  1.00  2.00           C
ATOM   2045  CG  ARG B 698      39.962   1.672   8.510  1.00  7.08           C
ATOM   2046  CD  ARG B 698      41.414   1.300   8.239  1.00 10.31           C
ATOM   2047  NE  ARG B 698      42.223   2.334   8.809  1.00 14.26           N
ATOM   2048  CZ  ARG B 698      42.863   3.260   8.137  1.00  9.60           C
ATOM   2049  NH1 ARG B 698      42.877   3.272   6.818  1.00  8.71           N
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ATOM   2050  NH2 ARG B 698      43.498   4.171   8.817  1.00  5.51           N
ATOM   2051  C   ARG B 698      37.198   0.423  10.881  1.00  4.51           C
ATOM   2052  O   ARG B 698      36.474   0.785  11.830  1.00  5.73           O
ATOM   2053  N   HIS B 699      37.445  -0.843  10.687  1.00  4.24           N
ATOM   2054  CA  HIS B 699      36.758  -1.862  11.467  1.00  4.34           C
ATOM   2055  CB  HIS B 699      36.070  -2.833  10.451  1.00  4.52           C
ATOM   2056  CG  HIS B 699      35.058  -3.760  11.034  1.00  2.22           C
ATOM   2057  ND1 HIS B 699      35.386  -4.729  11.964  1.00  3.86           N
ATOM   2058  CE1 HIS B 699      34.311  -5.460  12.229  1.00  2.00           C
ATOM   2059  NE2 HIS B 699      33.306  -5.005  11.507  1.00  2.00           N
ATOM   2060  CD2 HIS B 699      33.746  -3.935  10.758  1.00  2.00           C
ATOM   2061  C   HIS B 699      37.706  -2.621  12.402  1.00  3.78           C
ATOM   2062  O   HIS B 699      38.796  -2.946  12.041  1.00  2.51           O
ATOM   2063  N   LEU B 700      37.226  -2.906  13.608  1.00  3.99           N
ATOM   2064  CA  LEU B 700      37.962  -3.652  14.592  1.00  4.35           C
ATOM   2065  CB  LEU B 700      37.015  -4.031  15.713  1.00  3.43           C
ATOM   2066  CG  LEU B 700      37.467  -4.058  17.177  1.00  2.71           C
ATOM   2067  CD1 LEU B 700      36.714  -5.193  17.919  1.00  2.00           C
ATOM   2068  CD2 LEU B 700      38.954  -4.198  17.322  1.00  2.00           C
ATOM   2069  C   LEU B 700      38.512  -4.994  14.019  1.00  4.85           C
ATOM   2070  O   LEU B 700      39.607  -5.385  14.340  1.00  3.57           O
ATOM   2071  N   ASP B 701      37.737  -5.695  13.188  1.00  4.86           N
ATOM   2072  CA  ASP B 701      38.202  -6.958  12.691  1.00  5.27           C
ATOM   2073  CB  ASP B 701      37.055  -7.724  12.051  1.00  6.51           C
ATOM   2074  CG  ASP B 701      35.965  -8.161  13.051  1.00  8.63           C
ATOM   2075  OD1 ASP B 701      36.140  -8.095  14.300  1.00  8.97           O
ATOM   2076  OD2 ASP B 701      34.860  -8.568  12.634  1.00 12.11           O
ATOM   2077  C   ASP B 701      39.392  -6.779  11.683  1.00  5.92           C
ATOM   2078  O   ASP B 701      40.241  -7.654  11.524  1.00  4.87           O
ATOM   2079  N   GLN B 702      39.449  -5.650  10.990  1.00  6.01           N
ATOM   2080  CA  GLN B 702      40.548  -5.398  10.068  1.00  6.04           C
ATOM   2081  CB  GLN B 702      40.262  -4.162   9.205  1.00  5.99           C
ATOM   2082  CG  GLN B 702      38.897  -4.192   8.644  1.00  5.27           C
ATOM   2083  CD  GLN B 702      38.418  -2.903   8.079  1.00  4.96           C
ATOM   2084  OE1 GLN B 702      38.869  -1.797   8.471  1.00  4.27           O
ATOM   2085  NE2 GLN B 702      37.475  -3.020   7.135  1.00  3.80           N
ATOM   2086  C   GLN B 702      41.896  -5.243  10.829  1.00  6.46           C
ATOM   2087  O   GLN B 702      42.908  -5.756  10.357  1.00  6.12           O
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ATOM	2088	N	ILE B 703	41.899	-4.594	12.002	1.00	5.52	N
ATOM	2089	CA	ILE B 703	43.105	-4.450	12.777	1.00	6.51	C
ATOM	2090	CB	ILE B 703	42.911	-3.462	13.974	1.00	8.27	C
ATOM	2091	CG1	ILE B 703	43.146	-2.006	13.577	1.00	7.52	C
ATOM	2092	CD1	ILE B 703	42.183	-1.541	12.512	1.00	10.76	C
ATOM	2093	CG2	ILE B 703	43.838	-3.807	15.102	1.00	5.38	C
ATOM	2094	C	ILE B 703	43.451	-5.788	13.382	1.00	8.35	C
ATOM	2095	O	ILE B 703	44.630	-6.094	13.568	1.00	9.15	O
ATOM	2096	N	MET B 704	42.427	-6.586	13.720	1.00	8.61	N
ATOM	2097	CA	MET B 704	42.616	-7.906	14.325	1.00	7.76	C
ATOM	2098	CB	MET B 704	41.284	-8.558	14.722	1.00	7.41	C
ATOM	2099	CG	MET B 704	41.418	-9.941	15.451	1.00	9.47	C
ATOM	2100	SD	MET B 704	39.832	-10.902	15.795	1.00	8.72	S
ATOM	2101	CE	MET B 704	39.200	-10.805	14.093	1.00	2.92	C
ATOM	2102	C	MET B 704	43.363	-8.835	13.393	1.00	7.58	C
ATOM	2103	O	MET B 704	44.404	-9.378	13.736	1.00	8.07	O
ATOM	2104	N	MET B 705	42.825	-9.041	12.207	1.00	7.84	N
ATOM	2105	CA	MET B 705	43.404	-9.988	11.262	1.00	7.60	C
ATOM	2106	CB	MET B 705	42.471	-10.153	10.059	1.00	8.87	C
ATOM	2107	CG	MET B 705	41.137	-10.805	10.290	1.00	7.32	C
ATOM	2108	SD	MET B 705	40.198	-10.798	8.683	1.00	14.24	S
ATOM	2109	CE	MET B 705	39.124	-9.281	8.938	1.00	11.08	C
ATOM	2110	C	MET B 705	44.763	-9.464	10.826	1.00	8.08	C
ATOM	2111	O	MET B 705	45.637	-10.222	10.558	1.00	7.47	O
ATOM	2112	N	CYS B 706	44.936	-8.142	10.802	1.00	9.02	N
ATOM	2113	CA	CYS B 706	46.226	-7.550	10.487	1.00	9.66	C
ATOM	2114	CB	CYS B 706	46.091	-6.052	10.175	1.00	8.53	C
ATOM	2115	SG	CYS B 706	45.622	-5.697	8.466	1.00	10.44	S
ATOM	2116	C	CYS B 706	47.299	-7.794	11.592	1.00	10.66	C
ATOM	2117	O	CYS B 706	48.520	-7.837	11.297	1.00	10.39	O
ATOM	2118	N	SER B 707	46.870	-7.931	12.848	1.00	9.97	N
ATOM	2119	CA	SER B 707	47.837	-8.169	13.873	1.00	10.40	C
ATOM	2120	CB	SER B 707	47.296	-7.823	15.246	1.00	10.36	C
ATOM	2121	OG	SER B 707	47.061	-6.435	15.460	1.00	8.24	O
ATOM	2122	C	SER B 707	48.273	-9.654	13.807	1.00	12.62	C
ATOM	2123	O	SER B 707	49.474	-9.959	13.991	1.00	11.29	O
ATOM	2124	N	MET B 708	47.321	-10.563	13.507	1.00	14.70	N
ATOM	2125	CA	MET B 708	47.649	-12.000	13.401	1.00	16.47	C

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ATOM   2126  CB  MET B 708      46.449 -12.858  13.083  1.00 16.13           C
ATOM   2127  CG  MET B 708      45.246 -12.592  13.968  1.00 17.64           C
ATOM   2128  SD  MET B 708      43.770 -13.570  13.497  1.00 19.35           S
ATOM   2129  CE  MET B 708      44.439 -15.271  13.483  1.00 14.93           C
ATOM   2130  C   MET B 708      48.674 -12.174  12.299  1.00 18.00           C
ATOM   2131  O   MET B 708      49.789 -12.726  12.501  1.00 19.56           O
ATOM   2132  N   TYR B 709      48.316 -11.675  11.129  1.00 18.18           N
ATOM   2133  CA  TYR B 709      49.206 -11.742   9.981  1.00 18.22           C
ATOM   2134  CB  TYR B 709      48.600 -11.027   8.799  1.00 18.00           C
ATOM   2135  CG  TYR B 709      49.392 -11.215   7.533  1.00 20.73           C
ATOM   2136  CD1 TYR B 709      49.134 -12.285   6.686  1.00 20.65           C
ATOM   2137  CE1 TYR B 709      49.811 -12.431   5.520  1.00 22.80           C
ATOM   2138  CZ  TYR B 709      50.778 -11.520   5.187  1.00 23.73           C
ATOM   2139  OH  TYR B 709      51.492 -11.706   4.041  1.00 23.11           O
ATOM   2140  CE2 TYR B 709      51.062 -10.456   6.013  1.00 22.99           C
ATOM   2141  CD2 TYR B 709      50.372 -10.300   7.161  1.00 21.61           C
ATOM   2142  C   TYR B 709      50.587 -11.163  10.224  1.00 17.84           C
ATOM   2143  O   TYR B 709      51.559 -11.656   9.676  1.00 17.96           O
ATOM   2144  N   GLY B 710      50.665 -10.107  11.024  1.00 17.95           N
ATOM   2145  CA  GLY B 710      51.936  -9.469  11.349  1.00 17.36           C
ATOM   2146  C   GLY B 710      52.857 -10.280  12.271  1.00 17.08           C
ATOM   2147  O   GLY B 710      53.937 -10.643  11.848  1.00 18.01           O
ATOM   2148  N   ILE B 711      52.444 -10.585  13.493  1.00 16.32           N
ATOM   2149  CA  ILE B 711      53.288 -11.312  14.417  1.00 16.83           C
ATOM   2150  CB  ILE B 711      52.598 -11.494  15.796  1.00 15.62           C
ATOM   2151  CG1 ILE B 711      53.286 -10.673  16.876  1.00 17.22           C
ATOM   2152  CD1 ILE B 711      53.453  -9.239  16.632  1.00 18.82           C
ATOM   2153  CG2 ILE B 711      52.745 -12.930  16.319  1.00 13.88           C
ATOM   2154  C   ILE B 711      53.705 -12.666  13.783  1.00 18.91           C
ATOM   2155  O   ILE B 711      54.827 -13.122  13.926  1.00 17.41           O
ATOM   2156  N   CYS B 712      52.808 -13.303  13.049  1.00 20.88           N
ATOM   2157  CA  CYS B 712      53.214 -14.544  12.455  1.00 23.68           C
ATOM   2158  CB  CYS B 712      52.091 -15.179  11.615  1.00 23.93           C
ATOM   2159  SG  CYS B 712      50.569 -15.723  12.496  1.00 26.62           S
ATOM   2160  C   CYS B 712      54.430 -14.237  11.571  1.00 25.43           C
ATOM   2161  O   CYS B 712      55.390 -15.029  11.516  1.00 25.92           O
ATOM   2162  N   LYS B 713      54.392 -13.097  10.875  1.00 26.01           N
ATOM   2163  CA  LYS B 713      55.467 -12.746   9.970  1.00 27.09           C
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ATOM   2164  CB  LYS B 713      55.171 -11.436   9.272  1.00 27.73           C
ATOM   2165  CG  LYS B 713      54.261 -11.607   8.055  1.00 31.65           C
ATOM   2166  CD  LYS B 713      54.847 -12.565   7.008  1.00 35.08           C
ATOM   2167  CE  LYS B 713      54.103 -12.463   5.640  1.00 37.06           C
ATOM   2168  NZ  LYS B 713      54.896 -13.092   4.488  1.00 37.63           N
ATOM   2169  C   LYS B 713      56.825 -12.677  10.631  1.00 26.49           C
ATOM   2170  O   LYS B 713      57.790 -13.241  10.157  1.00 25.93           O
ATOM   2171  N   VAL B 714      56.900 -11.968  11.736  1.00 26.93           N
ATOM   2172  CA  VAL B 714      58.181 -11.816  12.437  1.00 26.50           C
ATOM   2173  CB  VAL B 714      58.141 -10.659  13.427  1.00 26.43           C
ATOM   2174  CG1 VAL B 714      58.139  -9.365  12.651  1.00 27.09           C
ATOM   2175  CG2 VAL B 714      56.913 -10.776  14.334  1.00 23.75           C
ATOM   2176  C   VAL B 714      58.631 -13.072  13.160  1.00 26.16           C
ATOM   2177  O   VAL B 714      59.795 -13.206  13.464  1.00 26.08           O
ATOM   2178  N   LYS B 715      57.697 -13.978  13.431  1.00 26.17           N
ATOM   2179  CA  LYS B 715      58.000 -15.241  14.067  1.00 26.40           C
ATOM   2180  CB  LYS B 715      56.935 -15.601  15.080  1.00 25.70           C
ATOM   2181  CG  LYS B 715      56.793 -14.644  16.220  1.00 23.21           C
ATOM   2182  CD  LYS B 715      57.950 -14.735  17.093  1.00 22.85           C
ATOM   2183  CE  LYS B 715      57.613 -14.356  18.501  1.00 21.73           C
ATOM   2184  NZ  LYS B 715      58.799 -14.669  19.392  1.00 20.20           N
ATOM   2185  C   LYS B 715      58.099 -16.343  13.008  1.00 28.00           C
ATOM   2186  O   LYS B 715      58.119 -17.523  13.325  1.00 27.94           O
ATOM   2187  N   ASN B 716      58.164 -15.941  11.749  1.00 29.90           N
ATOM   2188  CA  ASN B 716      58.255 -16.882  10.639  1.00 32.18           C
ATOM   2189  CB  ASN B 716      59.663 -17.488  10.599  1.00 33.07           C
ATOM   2190  CG  ASN B 716      60.627 -16.647   9.764  1.00 34.01           C
ATOM   2191  OD1 ASN B 716      61.153 -15.622  10.234  1.00 36.77           O
ATOM   2192  ND2 ASN B 716      60.847 -17.067   8.516  1.00 30.24           N
ATOM   2193  C   ASN B 716      57.185 -17.991  10.504  1.00 32.52           C
ATOM   2194  O   ASN B 716      57.395 -18.965   9.773  1.00 32.68           O
ATOM   2195  N   ILE B 717      56.060 -17.846  11.204  1.00 32.92           N
ATOM   2196  CA  ILE B 717      54.983 -18.826  11.142  1.00 32.59           C
ATOM   2197  CB  ILE B 717      54.031 -18.641  12.311  1.00 32.11           C
ATOM   2198  CG1 ILE B 717      54.799 -18.778  13.620  1.00 32.42           C
ATOM   2199  CD1 ILE B 717      55.411 -20.122  13.859  1.00 31.30           C
ATOM   2200  CG2 ILE B 717      52.865 -19.624  12.222  1.00 31.23           C
ATOM   2201  C   ILE B 717      54.251 -18.581   9.860  1.00 33.04           C
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ATOM   2202  O   ILE B 717      53.776 -17.477   9.616  1.00 34.05           O
ATOM   2203  N   ASP B 718      54.148 -19.604   9.035  1.00 33.06           N
ATOM   2204  CA  ASP B 718      53.501 -19.452   7.739  1.00 33.60           C
ATOM   2205  CB  ASP B 718      53.906 -20.614   6.831  1.00 33.73           C
ATOM   2206  CG  ASP B 718      53.353 -20.482   5.434  1.00 34.30           C
ATOM   2207  OD1 ASP B 718      53.839 -19.601   4.661  1.00 32.07           O
ATOM   2208  OD2 ASP B 718      52.432 -21.237   5.035  1.00 33.96           O
ATOM   2209  C   ASP B 718      51.974 -19.329   7.795  1.00 33.35           C
ATOM   2210  O   ASP B 718      51.249 -20.326   7.935  1.00 34.12           O
ATOM   2211  N   LEU B 719      51.469 -18.114   7.672  1.00 32.76           N
ATOM   2212  CA  LEU B 719      50.012 -17.908   7.748  1.00 32.36           C
ATOM   2213  CB  LEU B 719      49.590 -17.409   9.138  1.00 32.31           C
ATOM   2214  CG  LEU B 719      48.096 -17.110   9.353  1.00 33.01           C
ATOM   2215  CD1 LEU B 719      47.220 -18.253   8.871  1.00 31.76           C
ATOM   2216  CD2 LEU B 719      47.761 -16.776  10.820  1.00 32.06           C
ATOM   2217  C   LEU B 719      49.586 -16.934   6.682  1.00 31.40           C
ATOM   2218  O   LEU B 719      49.865 -15.743   6.764  1.00 30.98           O
ATOM   2219  N   LYS B 720      48.937 -17.454   5.664  1.00 30.94           N
ATOM   2220  CA  LYS B 720      48.521 -16.604   4.573  1.00 31.42           C
ATOM   2221  CB  LYS B 720      48.380 -17.419   3.278  1.00 31.88           C
ATOM   2222  CG  LYS B 720      49.634 -18.216   2.944  1.00 33.94           C
ATOM   2223  CD  LYS B 720      49.478 -19.008   1.649  1.00 37.89           C
ATOM   2224  CE  LYS B 720      49.501 -18.082   0.379  1.00 39.26           C
ATOM   2225  NZ  LYS B 720      49.418 -18.855  -0.944  1.00 38.62           N
ATOM   2226  C   LYS B 720      47.223 -15.858   4.896  1.00 30.27           C
ATOM   2227  O   LYS B 720      46.347 -16.374   5.592  1.00 30.09           O
ATOM   2228  N   PHE B 721      47.117 -14.644   4.368  1.00 29.04           N
ATOM   2229  CA  PHE B 721      45.957 -13.801   4.578  1.00 28.05           C
ATOM   2230  CB  PHE B 721      46.162 -12.422   3.958  1.00 28.24           C
ATOM   2231  CG  PHE B 721      46.005 -11.287   4.948  1.00 29.36           C
ATOM   2232  CD1 PHE B 721      44.870 -11.178   5.715  1.00 31.20           C
ATOM   2233  CE1 PHE B 721      44.728 -10.147   6.625  1.00 31.53           C
ATOM   2234  CZ  PHE B 721      45.750  -9.238   6.792  1.00 30.40           C
ATOM   2235  CE2 PHE B 721      46.885  -9.353   6.050  1.00 29.38           C
ATOM   2236  CD2 PHE B 721      47.017 -10.361   5.134  1.00 30.03           C
ATOM   2237  C   PHE B 721      44.714 -14.443   4.011  1.00 27.24           C
ATOM   2238  O   PHE B 721      43.614 -14.270   4.532  1.00 27.29           O
ATOM   2239  N   LYS B 722      44.888 -15.203   2.952  1.00 25.84           N
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ATOM   2240  CA  LYS B 722      43.762 -15.855   2.337  1.00 25.19           C
ATOM   2241  CB  LYS B 722      44.165 -16.442   0.986  1.00 26.12           C
ATOM   2242  CG  LYS B 722      43.008 -16.961   0.169  1.00 30.46           C
ATOM   2243  CD  LYS B 722      43.524 -17.782  -1.015  1.00 35.80           C
ATOM   2244  CE  LYS B 722      44.265 -19.065  -0.529  1.00 37.91           C
ATOM   2245  NZ  LYS B 722      43.363 -20.138  -0.003  1.00 36.85           N
ATOM   2246  C   LYS B 722      43.224 -16.916   3.276  1.00 23.23           C
ATOM   2247  O   LYS B 722      42.052 -17.236   3.235  1.00 23.64           O
ATOM   2248  N   ILE B 723      44.086 -17.465   4.117  1.00 21.64           N
ATOM   2249  CA  ILE B 723      43.670 -18.462   5.090  1.00 20.50           C
ATOM   2250  CB  ILE B 723      44.905 -19.242   5.626  1.00 20.86           C
ATOM   2251  CG1 ILE B 723      45.479 -20.194   4.560  1.00 22.30           C
ATOM   2252  CD1 ILE B 723      44.530 -21.368   4.187  1.00 25.70           C
ATOM   2253  CG2 ILE B 723      44.556 -20.036   6.895  1.00 18.10           C
ATOM   2254  C   ILE B 723      42.937 -17.771   6.249  1.00 19.81           C
ATOM   2255  O   ILE B 723      41.997 -18.301   6.822  1.00 20.17           O
ATOM   2256  N   ILE B 724      43.384 -16.581   6.600  1.00 17.88           N
ATOM   2257  CA  ILE B 724      42.789 -15.874   7.676  1.00 16.10           C
ATOM   2258  CB  ILE B 724      43.685 -14.687   8.034  1.00 16.51           C
ATOM   2259  CG1 ILE B 724      45.116 -15.191   8.240  1.00 13.98           C
ATOM   2260  CD1 ILE B 724      46.054 -14.177   8.828  1.00 13.32           C
ATOM   2261  CG2 ILE B 724      43.137 -13.949   9.255  1.00 16.09           C
ATOM   2262  C   ILE B 724      41.407 -15.432   7.288  1.00 15.97           C
ATOM   2263  O   ILE B 724      40.475 -15.523   8.079  1.00 15.53           O
ATOM   2264  N   VAL B 725      41.247 -14.975   6.058  1.00 16.45           N
ATOM   2265  CA  VAL B 725      39.946 -14.483   5.577  1.00 17.58           C
ATOM   2266  CB  VAL B 725      40.049 -14.015   4.145  1.00 18.51           C
ATOM   2267  CG1 VAL B 725      38.846 -14.384   3.410  1.00 19.37           C
ATOM   2268  CG2 VAL B 725      40.339 -12.541   4.079  1.00 20.64           C
ATOM   2269  C   VAL B 725      38.878 -15.563   5.615  1.00 17.09           C
ATOM   2270  O   VAL B 725      37.783 -15.368   6.169  1.00 17.94           O
ATOM   2271  N   THR B 726      39.216 -16.718   5.067  1.00 16.16           N
ATOM   2272  CA  THR B 726      38.304 -17.865   5.037  1.00 15.43           C
ATOM   2273  CB  THR B 726      38.983 -19.089   4.332  1.00 15.56           C
ATOM   2274  OG1 THR B 726      39.725 -18.634   3.194  1.00 15.24           O
ATOM   2275  CG2 THR B 726      37.963 -19.961   3.682  1.00 14.25           C
ATOM   2276  C   THR B 726      37.769 -18.254   6.428  1.00 14.32           C
ATOM   2277  O   THR B 726      36.600 -18.612   6.590  1.00 13.74           O
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ATOM   2278  N   ALA B 727      38.621 -18.208   7.430  1.00 13.02           N
ATOM   2279  CA  ALA B 727      38.182 -18.547   8.785  1.00 12.57           C
ATOM   2280  CB  ALA B 727      39.394 -18.653   9.663  1.00 12.86           C
ATOM   2281  C   ALA B 727      37.235 -17.440   9.331  1.00 12.91           C
ATOM   2282  O   ALA B 727      36.101 -17.702   9.745  1.00 11.86           O
ATOM   2283  N   TYR B 728      37.716 -16.195   9.289  1.00 13.37           N
ATOM   2284  CA  TYR B 728      36.915 -15.040   9.660  1.00 13.34           C
ATOM   2285  CB  TYR B 728      37.560 -13.739   9.134  1.00 12.87           C
ATOM   2286  CG  TYR B 728      36.773 -12.497   9.455  1.00 11.24           C
ATOM   2287  CD1 TYR B 728      36.790 -11.930  10.738  1.00  9.80           C
ATOM   2288  CE1 TYR B 728      36.061 -10.794  11.018  1.00  5.74           C
ATOM   2289  CZ  TYR B 728      35.323 -10.222  10.030  1.00  7.00           C
ATOM   2290  OH  TYR B 728      34.579  -9.074  10.272  1.00  7.47           O
ATOM   2291  CE2 TYR B 728      35.308 -10.766   8.777  1.00  5.96           C
ATOM   2292  CD2 TYR B 728      36.036 -11.875   8.493  1.00  7.33           C
ATOM   2293  C   TYR B 728      35.496 -15.203   9.111  1.00 13.39           C
ATOM   2294  O   TYR B 728      34.562 -15.001   9.856  1.00 12.47           O
ATOM   2295  N   LYS B 729      35.355 -15.598   7.831  1.00 13.99           N
ATOM   2296  CA  LYS B 729      34.034 -15.706   7.199  1.00 15.28           C
ATOM   2297  CB  LYS B 729      34.085 -16.311   5.783  1.00 14.79           C
ATOM   2298  CG  LYS B 729      34.768 -15.480   4.748  1.00 18.29           C
ATOM   2299  CD  LYS B 729      34.356 -15.844   3.278  1.00 21.11           C
ATOM   2300  CE  LYS B 729      35.021 -17.144   2.752  1.00 25.75           C
ATOM   2301  NZ  LYS B 729      34.801 -18.458   3.578  1.00 24.25           N
ATOM   2302  C   LYS B 729      33.100 -16.568   8.043  1.00 15.73           C
ATOM   2303  O   LYS B 729      31.884 -16.377   7.977  1.00 14.88           O
ATOM   2304  N   ASP B 730      33.659 -17.558   8.770  1.00 16.21           N
ATOM   2305  CA  ASP B 730      32.847 -18.411   9.671  1.00 17.14           C
ATOM   2306  CB  ASP B 730      33.624 -19.640  10.136  1.00 17.31           C
ATOM   2307  CG  ASP B 730      33.778 -20.688   9.036  1.00 20.23           C
ATOM   2308  OD1 ASP B 730      32.778 -20.962   8.350  1.00 22.19           O
ATOM   2309  OD2 ASP B 730      34.856 -21.298   8.810  1.00 20.06           O
ATOM   2310  C   ASP B 730      32.241 -17.690  10.914  1.00 16.31           C
ATOM   2311  O   ASP B 730      31.219 -18.118  11.429  1.00 17.05           O
ATOM   2312  N   LEU B 731      32.844 -16.610  11.392  1.00 14.65           N
ATOM   2313  CA  LEU B 731      32.243 -15.945  12.522  1.00 15.22           C
ATOM   2314  CB  LEU B 731      33.125 -14.789  13.052  1.00 14.75           C
ATOM   2315  CG  LEU B 731      34.636 -15.126  13.196  1.00 13.31           C
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ATOM   2316  CD1 LEU B 731      35.586 -13.937  13.501  1.00  8.91           C
ATOM   2317  CD2 LEU B 731      34.775 -16.150  14.223  1.00 11.15           C
ATOM   2318  C   LEU B 731      30.846 -15.507  12.109  1.00 15.53           C
ATOM   2319  O   LEU B 731      30.649 -15.085  10.986  1.00 15.48           O
ATOM   2320  N   PRO B 732      29.874 -15.635  13.008  1.00 16.47           N
ATOM   2321  CA  PRO B 732      28.444 -15.313  12.714  1.00 17.37           C
ATOM   2322  CB  PRO B 732      27.732 -15.685  14.022  1.00 17.22           C
ATOM   2323  CG  PRO B 732      28.872 -15.595  15.072  1.00 16.47           C
ATOM   2324  CD  PRO B 732      30.066 -16.164  14.367  1.00 15.27           C
ATOM   2325  C   PRO B 732      28.075 -13.853  12.326  1.00 18.51           C
ATOM   2326  O   PRO B 732      27.003 -13.592  11.762  1.00 17.81           O
ATOM   2327  N   HIS B 733      28.931 -12.894  12.620  1.00 19.79           N
ATOM   2328  CA  HIS B 733      28.578 -11.520  12.293  1.00 21.62           C
ATOM   2329  CB  HIS B 733      28.964 -10.622  13.462  1.00 22.24           C
ATOM   2330  CG  HIS B 733      30.392 -10.792  13.863  1.00 26.72           C
ATOM   2331  ND1 HIS B 733      31.403  -9.962  13.400  1.00 31.50           N
ATOM   2332  CE1 HIS B 733      32.566 -10.387  13.870  1.00 31.30           C
ATOM   2333  NE2 HIS B 733      32.343 -11.463  14.614  1.00 32.86           N
ATOM   2334  CD2 HIS B 733      30.998 -11.751  14.608  1.00 28.05           C
ATOM   2335  C   HIS B 733      29.366 -11.070  11.077  1.00 21.53           C
ATOM   2336  O   HIS B 733      29.161  -9.967  10.568  1.00 22.67           O
ATOM   2337  N   ALA B 734      30.276 -11.924  10.626  1.00 20.57           N
ATOM   2338  CA  ALA B 734      31.179 -11.610   9.525  1.00 19.72           C
ATOM   2339  CB  ALA B 734      32.132 -12.798   9.274  1.00 19.49           C
ATOM   2340  C   ALA B 734      30.555 -11.198   8.210  1.00 18.53           C
ATOM   2341  O   ALA B 734      29.738 -11.898   7.666  1.00 18.10           O
ATOM   2342  N   VAL B 735      31.036 -10.096   7.676  1.00 18.27           N
ATOM   2343  CA  VAL B 735      30.646  -9.624   6.357  1.00 18.38           C
ATOM   2344  CB  VAL B 735      30.027  -8.272   6.466  1.00 17.76           C
ATOM   2345  CG1 VAL B 735      29.805  -7.694   5.093  1.00 19.37           C
ATOM   2346  CG2 VAL B 735      28.741  -8.437   7.141  1.00 17.16           C
ATOM   2347  C   VAL B 735      31.832  -9.562   5.428  1.00 18.15           C
ATOM   2348  O   VAL B 735      32.839  -8.983   5.751  1.00 18.71           O
ATOM   2349  N   GLN B 736      31.712 -10.129   4.245  1.00 19.52           N
ATOM   2350  CA  GLN B 736      32.851 -10.140   3.292  1.00 20.24           C
ATOM   2351  CB  GLN B 736      32.435 -10.691   1.937  1.00 21.49           C
ATOM   2352  CG  GLN B 736      32.023 -12.190   1.994  1.00 26.42           C
ATOM   2353  CD  GLN B 736      32.035 -12.854   0.580  1.00 30.92           C
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ATOM	2354	OE1	GLN	B	736	33.109	-13.248	0.047	1.00	30.86	O
ATOM	2355	NE2	GLN	B	736	30.851	-12.949	-0.024	1.00	30.08	N
ATOM	2356	C	GLN	B	736	33.517	-8.799	3.100	1.00	18.33	C
ATOM	2357	O	GLN	B	736	34.771	-8.694	3.090	1.00	19.47	O
ATOM	2358	N	GLU	B	737	32.672	-7.793	2.972	1.00	15.56	N
ATOM	2359	CA	GLU	B	737	33.095	-6.424	2.769	1.00	14.71	C
ATOM	2360	CB	GLU	B	737	31.857	-5.518	2.763	1.00	13.93	C
ATOM	2361	CG	GLU	B	737	32.132	-4.035	2.789	1.00	20.16	C
ATOM	2362	CD	GLU	B	737	30.887	-3.181	3.145	1.00	29.64	C
ATOM	2363	OE1	GLU	B	737	30.162	-3.607	4.089	1.00	34.03	O
ATOM	2364	OE2	GLU	B	737	30.615	-2.096	2.518	1.00	27.73	O
ATOM	2365	C	GLU	B	737	34.206	-5.959	3.756	1.00	13.09	C
ATOM	2366	O	GLU	B	737	35.063	-5.162	3.389	1.00	13.18	O
ATOM	2367	N	THR	B	738	34.224	-6.472	4.984	1.00	11.57	N
ATOM	2368	CA	THR	B	738	35.257	-6.065	5.951	1.00	10.08	C
ATOM	2369	CB	THR	B	738	34.999	-6.653	7.332	1.00	8.74	C
ATOM	2370	OG1	THR	B	738	33.648	-6.403	7.711	1.00	9.41	O
ATOM	2371	CG2	THR	B	738	35.757	-5.946	8.356	1.00	2.00	C
ATOM	2372	C	THR	B	738	36.728	-6.349	5.527	1.00	10.98	C
ATOM	2373	O	THR	B	738	37.616	-5.661	5.995	1.00	9.61	O
ATOM	2374	N	PHE	B	739	36.976	-7.314	4.634	1.00	12.04	N
ATOM	2375	CA	PHE	B	739	38.338	-7.514	4.109	1.00	13.84	C
ATOM	2376	CB	PHE	B	739	38.926	-8.893	4.455	1.00	13.62	C
ATOM	2377	CG	PHE	B	739	38.107	-10.029	3.986	1.00	14.17	C
ATOM	2378	CD1	PHE	B	739	38.063	-10.348	2.633	1.00	14.68	C
ATOM	2379	CE1	PHE	B	739	37.279	-11.414	2.175	1.00	12.99	C
ATOM	2380	CZ	PHE	B	739	36.511	-12.157	3.098	1.00	11.66	C
ATOM	2381	CE2	PHE	B	739	36.550	-11.832	4.439	1.00	12.82	C
ATOM	2382	CD2	PHE	B	739	37.348	-10.775	4.879	1.00	12.84	C
ATOM	2383	C	PHE	B	739	38.449	-7.259	2.590	1.00	15.45	C
ATOM	2384	O	PHE	B	739	39.537	-7.256	2.013	1.00	16.07	O
ATOM	2385	N	LYS	B	740	37.338	-7.031	1.912	1.00	16.42	N
ATOM	2386	CA	LYS	B	740	37.424	-6.723	0.479	1.00	16.15	C
ATOM	2387	CB	LYS	B	740	36.213	-7.289	-0.258	1.00	17.06	C
ATOM	2388	CG	LYS	B	740	36.071	-8.841	-0.313	1.00	18.60	C
ATOM	2389	CD	LYS	B	740	35.364	-9.271	-1.631	1.00	17.32	C
ATOM	2390	CE	LYS	B	740	34.757	-10.655	-1.542	1.00	22.65	C
ATOM	2391	NZ	LYS	B	740	35.750	-11.740	-1.288	1.00	26.48	N

ATOM	2392	C	LYS	B	740	37.470	-5.213	0.201	1.00	15.61	C
ATOM	2393	O	LYS	B	740	37.968	-4.795	-0.822	1.00	14.70	O
ATOM	2394	N	ARG	B	741	36.920	-4.416	1.127	1.00	15.05	N
ATOM	2395	CA	ARG	B	741	36.797	-2.962	0.995	1.00	14.19	C
ATOM	2396	CB	ARG	B	741	35.330	-2.620	0.730	1.00	14.64	C
ATOM	2397	CG	ARG	B	741	35.008	-1.179	0.421	1.00	16.18	C
ATOM	2398	CD	ARG	B	741	33.588	-0.966	-0.148	1.00	24.70	C
ATOM	2399	NE	ARG	B	741	33.531	0.033	-1.252	1.00	25.41	N
ATOM	2400	CZ	ARG	B	741	33.785	1.342	-1.084	1.00	26.65	C
ATOM	2401	NH1	ARG	B	741	34.096	1.807	0.123	1.00	25.62	N
ATOM	2402	NH2	ARG	B	741	33.733	2.193	-2.102	1.00	25.67	N
ATOM	2403	C	ARG	B	741	37.245	-2.300	2.291	1.00	13.80	C
ATOM	2404	O	ARG	B	741	36.469	-2.118	3.199	1.00	12.81	O
ATOM	2405	N	VAL	B	742	38.519	-1.966	2.379	1.00	13.97	N
ATOM	2406	CA	VAL	B	742	39.089	-1.379	3.586	1.00	14.00	C
ATOM	2407	CB	VAL	B	742	40.197	-2.276	4.165	1.00	14.78	C
ATOM	2408	CG1	VAL	B	742	40.864	-1.627	5.411	1.00	12.67	C
ATOM	2409	CG2	VAL	B	742	39.671	-3.683	4.413	1.00	13.17	C
ATOM	2410	C	VAL	B	742	39.698	-0.039	3.193	1.00	13.99	C
ATOM	2411	O	VAL	B	742	40.175	0.101	2.069	1.00	13.44	O
ATOM	2412	N	LEU	B	743	39.640	0.928	4.096	1.00	14.08	N
ATOM	2413	CA	LEU	B	743	40.118	2.281	3.834	1.00	16.23	C
ATOM	2414	CB	LEU	B	743	39.695	3.196	4.950	1.00	16.17	C
ATOM	2415	CG	LEU	B	743	39.291	4.624	4.687	1.00	17.47	C
ATOM	2416	CD1	LEU	B	743	39.320	5.415	5.988	1.00	16.65	C
ATOM	2417	CD2	LEU	B	743	40.177	5.284	3.687	1.00	19.65	C
ATOM	2418	C	LEU	B	743	41.622	2.365	3.695	1.00	17.49	C
ATOM	2419	O	LEU	B	743	42.360	1.710	4.400	1.00	17.60	O
ATOM	2420	N	ILE	B	744	42.072	3.160	2.744	1.00	20.53	N
ATOM	2421	CA	ILE	B	744	43.492	3.338	2.533	1.00	23.74	C
ATOM	2422	CB	ILE	B	744	43.902	2.930	1.102	1.00	24.04	C
ATOM	2423	CG1	ILE	B	744	43.379	1.514	0.756	1.00	22.67	C
ATOM	2424	CD1	ILE	B	744	43.896	0.426	1.560	1.00	19.74	C
ATOM	2425	CG2	ILE	B	744	45.405	2.990	0.952	1.00	23.62	C
ATOM	2426	C	ILE	B	744	43.982	4.733	2.819	1.00	25.89	C
ATOM	2427	O	ILE	B	744	44.797	4.898	3.691	1.00	26.76	O
ATOM	2428	N	LYS	B	745	43.493	5.737	2.100	1.00	28.94	N
ATOM	2429	CA	LYS	B	745	44.043	7.102	2.253	1.00	31.98	C

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ATOM   2430  CB  LYS B 745      44.911   7.474   1.035  1.00 31.99      C
ATOM   2431  CG  LYS B 745      46.346   6.997   1.095  1.00 33.87      C
ATOM   2432  CD  LYS B 745      46.918   6.683  -0.307  1.00 35.93      C
ATOM   2433  CE  LYS B 745      47.283   7.943  -1.086  1.00 33.52      C
ATOM   2434  NZ  LYS B 745      46.120   8.507  -1.826  1.00 32.74      N
ATOM   2435  C   LYS B 745      43.011   8.218   2.510  1.00 33.73      C
ATOM   2436  O   LYS B 745      43.033   8.889   3.574  1.00 35.26      O
ATOM   2437  N   GLU B 746      42.125   8.457   1.542  1.00 34.28      N
ATOM   2438  CA  GLU B 746      41.094   9.456   1.767  1.00 35.03      C
ATOM   2439  CB  GLU B 746      41.370  10.733   0.995  1.00 35.68      C
ATOM   2440  CG  GLU B 746      41.647  10.472  -0.457  1.00 39.53      C
ATOM   2441  CD  GLU B 746      42.782   9.502  -0.614  1.00 42.55      C
ATOM   2442  OE1 GLU B 746      43.920   9.880  -0.281  1.00 42.51      O
ATOM   2443  OE2 GLU B 746      42.519   8.364  -1.034  1.00 47.78      O
ATOM   2444  C   GLU B 746      39.726   8.925   1.439  1.00 34.47      C
ATOM   2445  O   GLU B 746      38.844   8.974   2.266  1.00 36.86      O
ATOM   2446  N   GLU B 747      39.526   8.424   0.234  1.00 33.35      N
ATOM   2447  CA  GLU B 747      38.245   7.839  -0.115  1.00 31.94      C
ATOM   2448  CB  GLU B 747      37.426   8.821  -0.936  1.00 32.95      C
ATOM   2449  CG  GLU B 747      37.090  10.125  -0.212  1.00 36.33      C
ATOM   2450  CD  GLU B 747      35.781  10.735  -0.705  1.00 39.89      C
ATOM   2451  OE1 GLU B 747      34.720  10.153  -0.373  1.00 39.59      O
ATOM   2452  OE2 GLU B 747      35.812  11.772  -1.431  1.00 40.99      O
ATOM   2453  C   GLU B 747      38.504   6.586  -0.928  1.00 30.15      C
ATOM   2454  O   GLU B 747      37.614   6.091  -1.625  1.00 29.18      O
ATOM   2455  N   GLU B 748      39.747   6.109  -0.820  1.00 28.29      N
ATOM   2456  CA  GLU B 748      40.251   4.934  -1.509  1.00 27.13      C
ATOM   2457  CB  GLU B 748      41.666   5.225  -2.007  1.00 27.78      C
ATOM   2458  CG  GLU B 748      42.369   4.026  -2.600  1.00 31.92      C
ATOM   2459  CD  GLU B 748      41.560   3.391  -3.728  1.00 39.42      C
ATOM   2460  OE1 GLU B 748      40.892   4.135  -4.511  1.00 41.77      O
ATOM   2461  OE2 GLU B 748      41.576   2.138  -3.828  1.00 41.89      O
ATOM   2462  C   GLU B 748      40.192   3.607  -0.701  1.00 25.04      C
ATOM   2463  O   GLU B 748      40.724   3.480   0.411  1.00 23.53      O
ATOM   2464  N   TYR B 749      39.506   2.621  -1.270  1.00 23.64      N
ATOM   2465  CA  TYR B 749      39.390   1.305  -0.645  1.00 21.89      C
ATOM   2466  CB  TYR B 749      37.939   1.027  -0.350  1.00 21.59      C
ATOM   2467  CG  TYR B 749      37.363   1.979   0.662  1.00 19.85      C
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ATOM   2468  CD1 TYR B 749      37.125   3.290   0.327  1.00 17.50      C
ATOM   2469  CE1 TYR B 749      36.596   4.167   1.231  1.00 19.14      C
ATOM   2470  CZ  TYR B 749      36.300   3.745   2.506  1.00 19.16      C
ATOM   2471  OH  TYR B 749      35.764   4.657   3.419  1.00 18.64      O
ATOM   2472  CE2 TYR B 749      36.536   2.427   2.857  1.00 19.01      C
ATOM   2473  CD2 TYR B 749      37.063   1.563   1.946  1.00 17.38      C
ATOM   2474  C   TYR B 749      39.964   0.192  -1.504  1.00 20.89      C
ATOM   2475  O   TYR B 749      39.916   0.259  -2.716  1.00 21.97      O
ATOM   2476  N   ASP B 750      40.494  -0.837  -0.866  1.00 20.13      N
ATOM   2477  CA  ASP B 750      41.111  -1.970  -1.538  1.00 18.82      C
ATOM   2478  CB  ASP B 750      42.567  -1.679  -1.874  1.00 19.07      C
ATOM   2479  CG  ASP B 750      42.941  -2.117  -3.312  1.00 20.57      C
ATOM   2480  OD1 ASP B 750      42.687  -3.314  -3.677  1.00 15.59      O
ATOM   2481  OD2 ASP B 750      43.496  -1.299  -4.114  1.00 20.85      O
ATOM   2482  C   ASP B 750      41.067  -3.110  -0.580  1.00 17.86      C
ATOM   2483  O   ASP B 750      40.606  -2.927   0.545  1.00 18.20      O
ATOM   2484  N   SER B 751      41.534  -4.277  -1.023  1.00 16.66      N
ATOM   2485  CA  SER B 751      41.594  -5.478  -0.198  1.00 15.69      C
ATOM   2486  CB  SER B 751      42.277  -6.578  -0.976  1.00 14.91      C
ATOM   2487  OG  SER B 751      43.683  -6.392  -0.953  1.00 15.07      O
ATOM   2488  C   SER B 751      42.349  -5.264   1.138  1.00 15.52      C
ATOM   2489  O   SER B 751      43.138  -4.346   1.310  1.00 15.02      O
ATOM   2490  N   ILE B 752      42.142  -6.147   2.083  1.00 15.22      N
ATOM   2491  CA  ILE B 752      42.790  -5.968   3.367  1.00 15.33      C
ATOM   2492  CB  ILE B 752      42.236  -6.937   4.387  1.00 14.48      C
ATOM   2493  CG1 ILE B 752      42.606  -6.495   5.805  1.00 15.87      C
ATOM   2494  CD1 ILE B 752      41.941  -7.320   6.917  1.00 12.60      C
ATOM   2495  CG2 ILE B 752      42.760  -8.248   4.108  1.00 14.29      C
ATOM   2496  C   ILE B 752      44.295  -6.089   3.284  1.00 15.94      C
ATOM   2497  O   ILE B 752      44.984  -5.642   4.209  1.00 16.82      O
ATOM   2498  N   ILE B 753      44.803  -6.656   2.186  1.00 15.32      N
ATOM   2499  CA  ILE B 753      46.219  -6.847   2.011  1.00 15.05      C
ATOM   2500  CB  ILE B 753      46.481  -7.795   0.834  1.00 16.49      C
ATOM   2501  CG1 ILE B 753      46.016  -9.193   1.137  1.00 17.73      C
ATOM   2502  CD1 ILE B 753      45.975 -10.051  -0.111  1.00 17.48      C
ATOM   2503  CG2 ILE B 753      47.962  -7.928   0.502  1.00 17.13      C
ATOM   2504  C   ILE B 753      46.830  -5.512   1.672  1.00 14.92      C
ATOM   2505  O   ILE B 753      47.876  -5.155   2.189  1.00 15.50      O
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ATOM	2506	N	VAL	B	754	46.222	-4.772	0.756	1.00	14.19	N
ATOM	2507	CA	VAL	B	754	46.811	-3.490	0.387	1.00	13.27	C
ATOM	2508	CB	VAL	B	754	45.977	-2.757	-0.669	1.00	13.73	C
ATOM	2509	CG1	VAL	B	754	46.516	-1.366	-0.960	1.00	13.78	C
ATOM	2510	CG2	VAL	B	754	45.829	-3.593	-1.938	1.00	13.40	C
ATOM	2511	C	VAL	B	754	46.863	-2.657	1.656	1.00	13.15	C
ATOM	2512	O	VAL	B	754	47.807	-1.884	1.862	1.00	12.76	O
ATOM	2513	N	PHE	B	755	45.863	-2.832	2.528	1.00	12.25	N
ATOM	2514	CA	PHE	B	755	45.849	-2.081	3.763	1.00	11.74	C
ATOM	2515	CB	PHE	B	755	44.564	-2.286	4.554	1.00	12.24	C
ATOM	2516	CG	PHE	B	755	44.591	-1.641	5.917	1.00	9.65	C
ATOM	2517	CD1	PHE	B	755	44.648	-0.250	6.030	1.00	11.69	C
ATOM	2518	CE1	PHE	B	755	44.710	0.373	7.313	1.00	13.58	C
ATOM	2519	CZ	PHE	B	755	44.678	-0.431	8.444	1.00	12.16	C
ATOM	2520	CE2	PHE	B	755	44.603	-1.833	8.307	1.00	8.49	C
ATOM	2521	CD2	PHE	B	755	44.568	-2.414	7.070	1.00	5.62	C
ATOM	2522	C	PHE	B	755	47.028	-2.440	4.638	1.00	11.89	C
ATOM	2523	O	PHE	B	755	47.725	-1.554	5.142	1.00	10.64	O
ATOM	2524	N	TYR	B	756	47.239	-3.741	4.848	1.00	12.44	N
ATOM	2525	CA	TYR	B	756	48.369	-4.170	5.674	1.00	13.71	C
ATOM	2526	CB	TYR	B	756	48.450	-5.675	5.721	1.00	13.48	C
ATOM	2527	CG	TYR	B	756	49.697	-6.181	6.414	1.00	16.30	C
ATOM	2528	CD1	TYR	B	756	49.792	-6.197	7.793	1.00	16.18	C
ATOM	2529	CE1	TYR	B	756	50.933	-6.683	8.441	1.00	18.26	C
ATOM	2530	CZ	TYR	B	756	52.012	-7.161	7.687	1.00	21.98	C
ATOM	2531	OH	TYR	B	756	53.166	-7.628	8.297	1.00	17.21	O
ATOM	2532	CE2	TYR	B	756	51.935	-7.156	6.293	1.00	20.27	C
ATOM	2533	CD2	TYR	B	756	50.782	-6.674	5.673	1.00	20.75	C
ATOM	2534	C	TYR	B	756	49.688	-3.564	5.123	1.00	14.37	C
ATOM	2535	O	TYR	B	756	50.386	-2.764	5.791	1.00	14.12	O
ATOM	2536	N	ASN	B	757	49.988	-3.880	3.867	1.00	14.19	N
ATOM	2537	CA	ASN	B	757	51.213	-3.374	3.300	1.00	15.33	C
ATOM	2538	CB	ASN	B	757	51.516	-4.070	1.984	1.00	15.54	C
ATOM	2539	CG	ASN	B	757	51.770	-5.537	2.177	1.00	18.19	C
ATOM	2540	OD1	ASN	B	757	52.778	-5.936	2.783	1.00	19.68	O
ATOM	2541	ND2	ASN	B	757	50.851	-6.363	1.680	1.00	20.50	N
ATOM	2542	C	ASN	B	757	51.320	-1.860	3.141	1.00	14.85	C
ATOM	2543	O	ASN	B	757	52.419	-1.337	3.198	1.00	15.14	O

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ATOM   2544  N   SER B 758      50.210  -1.162   2.942  1.00 13.60           N
ATOM   2545  CA  SER B 758      50.310   0.251   2.646  1.00 13.76           C
ATOM   2546  CB  SER B 758      49.283   0.667   1.603  1.00 13.54           C
ATOM   2547  OG  SER B 758      49.507  -0.024   0.387  1.00 15.82           O
ATOM   2548  C   SER B 758      50.167   1.178   3.823  1.00 14.24           C
ATOM   2549  O   SER B 758      50.628   2.331   3.727  1.00 14.50           O
ATOM   2550  N   VAL B 759      49.516   0.701   4.899  1.00 13.20           N
ATOM   2551  CA  VAL B 759      49.204   1.515   6.035  1.00 12.81           C
ATOM   2552  CB  VAL B 759      47.751   1.834   6.030  1.00 12.98           C
ATOM   2553  CG1 VAL B 759      47.457   2.869   7.066  1.00 12.46           C
ATOM   2554  CG2 VAL B 759      47.378   2.343   4.650  1.00 13.50           C
ATOM   2555  C   VAL B 759      49.558   0.906   7.375  1.00 14.10           C
ATOM   2556  O   VAL B 759      50.245   1.528   8.144  1.00 14.24           O
ATOM   2557  N   PHE B 760      49.113  -0.320   7.641  1.00 14.78           N
ATOM   2558  CA  PHE B 760      49.305  -0.964   8.916  1.00 15.29           C
ATOM   2559  CB  PHE B 760      48.569  -2.314   8.884  1.00 15.21           C
ATOM   2560  CG  PHE B 760      48.414  -2.965  10.234  1.00 14.87           C
ATOM   2561  CD1 PHE B 760      47.385  -2.591  11.085  1.00 13.04           C
ATOM   2562  CE1 PHE B 760      47.237  -3.188  12.302  1.00 13.09           C
ATOM   2563  CZ  PHE B 760      48.118  -4.129  12.712  1.00 13.72           C
ATOM   2564  CE2 PHE B 760      49.165  -4.488  11.897  1.00 15.35           C
ATOM   2565  CD2 PHE B 760      49.304  -3.918  10.660  1.00 13.80           C
ATOM   2566  C   PHE B 760      50.785  -1.162   9.246  1.00 16.61           C
ATOM   2567  O   PHE B 760      51.333  -0.642  10.217  1.00 16.43           O
ATOM   2568  N   MET B 761      51.422  -1.954   8.426  1.00 18.47           N
ATOM   2569  CA  MET B 761      52.791  -2.303   8.631  1.00 21.12           C
ATOM   2570  CB  MET B 761      53.267  -3.148   7.451  1.00 22.42           C
ATOM   2571  CG  MET B 761      54.775  -3.092   7.205  1.00 24.52           C
ATOM   2572  SD  MET B 761      55.033  -4.025   5.779  1.00 32.46           S
ATOM   2573  CE  MET B 761      55.132  -5.783   6.464  1.00 33.08           C
ATOM   2574  C   MET B 761      53.689  -1.091   8.816  1.00 21.28           C
ATOM   2575  O   MET B 761      54.647  -1.132   9.533  1.00 22.18           O
ATOM   2576  N   GLN B 762      53.381  -0.005   8.159  1.00 22.50           N
ATOM   2577  CA  GLN B 762      54.223   1.171   8.259  1.00 22.90           C
ATOM   2578  CB  GLN B 762      53.913   2.123   7.106  1.00 23.18           C
ATOM   2579  CG  GLN B 762      53.783   1.393   5.714  1.00 27.77           C
ATOM   2580  CD  GLN B 762      55.041   0.617   5.279  1.00 32.36           C
ATOM   2581  OE1 GLN B 762      55.947   1.172   4.658  1.00 34.37           O
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ATOM   2582  NE2 GLN B 762      55.071  -0.687   5.585  1.00 36.21           N
ATOM   2583  C   GLN B 762      54.043   1.853   9.593  1.00 21.95           C
ATOM   2584  O   GLN B 762      54.985   2.236  10.247  1.00 21.06           O
ATOM   2585  N   ARG B 763      52.815   2.011  10.012  1.00 21.79           N
ATOM   2586  CA  ARG B 763      52.622   2.728  11.232  1.00 22.55           C
ATOM   2587  CB  ARG B 763      51.143   3.037  11.405  1.00 23.18           C
ATOM   2588  CG  ARG B 763      50.785   3.636  12.785  1.00 27.01           C
ATOM   2589  CD  ARG B 763      51.197   5.097  12.938  1.00 31.66           C
ATOM   2590  NE  ARG B 763      50.298   5.888  12.126  1.00 36.41           N
ATOM   2591  CZ  ARG B 763      49.055   6.188  12.498  1.00 39.77           C
ATOM   2592  NH1 ARG B 763      48.603   5.780  13.691  1.00 36.61           N
ATOM   2593  NH2 ARG B 763      48.273   6.913  11.691  1.00 40.01           N
ATOM   2594  C   ARG B 763      53.158   1.947  12.436  1.00 22.17           C
ATOM   2595  O   ARG B 763      53.538   2.537  13.438  1.00 19.77           O
ATOM   2596  N   LEU B 764      53.190   0.617  12.300  1.00 22.80           N
ATOM   2597  CA  LEU B 764      53.588  -0.269  13.386  1.00 23.24           C
ATOM   2598  CB  LEU B 764      52.500  -1.301  13.594  1.00 23.48           C
ATOM   2599  CG  LEU B 764      51.177  -0.718  14.097  1.00 24.36           C
ATOM   2600  CD1 LEU B 764      50.013  -1.676  13.885  1.00 24.21           C
ATOM   2601  CD2 LEU B 764      51.348  -0.480  15.529  1.00 24.26           C
ATOM   2602  C   LEU B 764      54.917  -0.993  13.193  1.00 23.50           C
ATOM   2603  O   LEU B 764      55.345  -1.716  14.089  1.00 21.69           O
ATOM   2604  N   LYS B 765      55.556  -0.812  12.032  1.00 24.54           N
ATOM   2605  CA  LYS B 765      56.800  -1.510  11.719  1.00 26.74           C
ATOM   2606  CB  LYS B 765      57.462  -0.944  10.464  1.00 26.88           C
ATOM   2607  CG  LYS B 765      58.915  -1.493  10.240  1.00 28.72           C
ATOM   2608  CD  LYS B 765      59.559  -1.044   8.915  1.00 31.45           C
ATOM   2609  CE  LYS B 765      58.982  -1.767   7.693  1.00 34.41           C
ATOM   2610  NZ  LYS B 765      57.496  -1.689   7.597  1.00 37.61           N
ATOM   2611  C   LYS B 765      57.796  -1.462  12.879  1.00 28.01           C
ATOM   2612  O   LYS B 765      58.254  -2.494  13.377  1.00 27.53           O
ATOM   2613  N   THR B 766      58.126  -0.242  13.273  1.00 29.05           N
ATOM   2614  CA  THR B 766      58.966   0.013  14.424  1.00 30.88           C
ATOM   2615  CB  THR B 766      58.821   1.516  14.840  1.00 31.26           C
ATOM   2616  OG1 THR B 766      59.035   2.348  13.698  1.00 33.49           O
ATOM   2617  CG2 THR B 766      59.909   1.962  15.802  1.00 30.65           C
ATOM   2618  C   THR B 766      58.615  -0.872  15.610  1.00 30.99           C
ATOM   2619  O   THR B 766      59.449  -1.569  16.119  1.00 32.43           O
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ATOM   2620  N   ASN B 767      57.398  -0.804  16.083  1.00 31.61           N
ATOM   2621  CA  ASN B 767.     56.992  -1.570  17.232  1.00 33.54           C
ATOM   2622  CB  ASN B 767      55.652  -1.023  17.768  1.00 33.93           C
ATOM   2623  CG  ASN B 767      55.048  -1.892  18.837  1.00 36.39           C
ATOM   2624  OD1 ASN B 767      54.504  -2.945  18.545  1.00 39.39           O
ATOM   2625  ND2 ASN B 767      55.142  -1.456  20.094  1.00 40.65           N
ATOM   2626  C   ASN B 767      56.926  -3.092  16.985  1.00 34.59           C
ATOM   2627  O   ASN B 767      57.394  -3.895  17.816  1.00 34.71           O
ATOM   2628  N   ILE B 768      56.354  -3.511  15.863  1.00 35.47           N
ATOM   2629  CA  ILE B 768      56.239  -4.940  15.625  1.00 36.32           C
ATOM   2630  CB  ILE B 768      55.621  -5.237  14.268  1.00 36.49           C
ATOM   2631  CG1 ILE B 768      54.105  -4.966  14.309  1.00 35.72           C
ATOM   2632  CD1 ILE B 768      53.429  -5.168  12.981  1.00 35.45           C
ATOM   2633  CG2 ILE B 768      55.950  -6.683  13.834  1.00 34.18           C
ATOM   2634  C   ILE B 768      57.592  -5.577  15.698  1.00 37.63           C
ATOM   2635  O   ILE B 768      57.694  -6.786  15.923  1.00 38.19           O
ATOM   2636  N   LEU B 769      58.626  -4.764  15.505  1.00 38.55           N
ATOM   2637  CA  LEU B 769      59.996  -5.257  15.523  1.00 40.19           C
ATOM   2638  CB  LEU B 769      60.996  -4.186  15.082  1.00 40.99           C
ATOM   2639  CG  LEU B 769      61.863  -4.615  13.896  1.00 42.49           C
ATOM   2640  CD1 LEU B 769      62.460  -5.984  14.251  1.00 45.30           C
ATOM   2641  CD2 LEU B 769      61.061  -4.723  12.578  1.00 42.90           C
ATOM   2642  C   LEU B 769      60.375  -5.753  16.890  1.00 40.93           C
ATOM   2643  O   LEU B 769      61.022  -6.789  16.999  1.00 41.56           O
ATOM   2644  N   GLN B 770      59.987  -5.024  17.936  1.00 41.51           N
ATOM   2645  CA  GLN B 770      60.285  -5.473  19.304  1.00 41.74           C
ATOM   2646  CB  GLN B 770      59.366  -4.794  20.343  1.00 41.53           C
ATOM   2647  CG  GLN B 770      59.450  -5.418  21.762  1.00 42.43           C
ATOM   2648  CD  GLN B 770      58.133  -5.425  22.587  1.00 42.74           C
ATOM   2649  OE1 GLN B 770      58.064  -6.041  23.668  1.00 41.16           O
ATOM   2650  NE2 GLN B 770      57.116  -4.740  22.090  1.00 43.74           N
ATOM   2651  C   GLN B 770      60.125  -7.004  19.380  1.00 41.82           C
ATOM   2652  O   GLN B 770      61.077  -7.747  19.610  1.00 41.81           O
ATOM   2653  N   TYR B 771      58.911  -7.467  19.144  1.00 42.24           N
ATOM   2654  CA  TYR B 771      58.610  -8.888  19.229  1.00 42.97           C
ATOM   2655  CB  TYR B 771      57.180  -9.140  18.775  1.00 41.87           C
ATOM   2656  CG  TYR B 771      56.175  -8.189  19.354  1.00 38.45           C
ATOM   2657  CD1 TYR B 771      55.729  -8.307  20.662  1.00 37.30           C
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ATOM	2658	CE1	TYR	B	771	54.776	-7.426	21.169	1.00 35.23	C
ATOM	2659	CZ	TYR	B	771	54.263	-6.431	20.343	1.00 34.31	C
ATOM	2660	OH	TYR	B	771	53.309	-5.491	20.752	1.00 34.71	O
ATOM	2661	CE2	TYR	B	771	54.703	-6.332	19.061	1.00 33.76	C
ATOM	2662	CD2	TYR	B	771	55.641	-7.191	18.576	1.00 35.17	C
ATOM	2663	C	TYR	B	771	59.572	-9.775	18.441	1.00 44.15	C
ATOM	2664	O	TYR	B	771	59.703	-10.968	18.720	1.00 43.36	O
ATOM	2665	N	ALA	B	772	60.235	-9.181	17.454	1.00 46.14	N
ATOM	2666	CA	ALA	B	772	61.159	-9.932	16.620	1.00 48.39	C
ATOM	2667	CB	ALA	B	772	61.590	-9.113	15.432	1.00 48.34	C
ATOM	2668	C	ALA	B	772	62.368	-10.356	17.425	1.00 50.30	C
ATOM	2669	O	ALA	B	772	62.956	-11.413	17.175	1.00 50.02	O
ATOM	2670	N	SER	B	773	62.746	-9.510	18.383	1.00 52.64	N
ATOM	2671	CA	SER	B	773	63.884	-9.794	19.238	1.00 54.66	C
ATOM	2672	CB	SER	B	773	64.021	-8.723	20.320	1.00 54.48	C
ATOM	2673	OG	SER	B	773	65.106	-9.024	21.187	1.00 55.08	O
ATOM	2674	C	SER	B	773	63.691	-11.173	19.879	1.00 56.17	C
ATOM	2675	O	SER	B	773	62.634	-11.447	20.455	1.00 56.55	O
ATOM	2676	N	THR	B	774	64.709	-12.031	19.768	1.00 57.80	N
ATOM	2677	CA	THR	B	774	64.694	-13.397	20.328	1.00 59.18	C
ATOM	2678	CB	THR	B	774	65.990	-14.164	19.901	1.00 59.51	C
ATOM	2679	OG1	THR	B	774	67.155	-13.432	20.324	1.00 60.23	O
ATOM	2680	CG2	THR	B	774	66.138	-14.219	18.355	1.00 59.89	C
ATOM	2681	C	THR	B	774	64.527	-13.436	21.875	1.00 59.52	C
ATOM	2682	O	THR	B	774	64.836	-14.440	22.533	1.00 59.47	O
ATOM	2683	N	ARG	B	775	64.043	-12.330	22.433	1.00 59.58	N
ATOM	2684	CA	ARG	B	775	63.800	-12.203	23.861	1.00 59.55	C
ATOM	2685	CB	ARG	B	775	64.540	-10.968	24.393	1.00 59.96	C
ATOM	2686	CG	ARG	B	775	64.053	-9.623	23.789	1.00 60.09	C
ATOM	2687	CD	ARG	B	775	64.791	-8.402	24.311	1.00 59.27	C
ATOM	2688	NE	ARG	B	775	64.233	-7.147	23.810	1.00 58.26	N
ATOM	2689	CZ	ARG	B	775	63.016	-6.685	24.091	1.00 57.54	C
ATOM	2690	NH1	ARG	B	775	62.186	-7.364	24.871	1.00 56.28	N
ATOM	2691	NH2	ARG	B	775	62.618	-5.532	23.577	1.00 57.23	N
ATOM	2692	C	ARG	B	775	62.283	-12.077	24.117	1.00 59.35	C
ATOM	2693	O	ARG	B	775	61.559	-11.452	23.327	1.00 59.00	O
ATOM	2694	N	PRO	B	776	61.799	-12.663	25.217	1.00 59.19	N
ATOM	2695	CA	PRO	B	776	60.358	-12.614	25.546	1.00 58.52	C

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ATOM   2696  CB  PRO B 776      60.263 -13.471  26.817  1.00 58.69           C
ATOM   2697  CG  PRO B 776      61.659 -13.372  27.413  1.00 59.27           C
ATOM   2698  CD  PRO B 776      62.577 -13.431  26.219  1.00 59.00           C
ATOM   2699  C   PRO B 776      59.846 -11.173  25.804  1.00 57.74           C
ATOM   2700  O   PRO B 776      60.560 -10.337  26.404  1.00 57.92           O
ATOM   2701  N   PRO B 777      58.638 -10.887  25.321  1.00 56.28           N
ATOM   2702  CA  PRO B 777      58.011  -9.569  25.464  1.00 55.27           C
ATOM   2703  CB  PRO B 777      57.078  -9.548  24.271  1.00 55.36           C
ATOM   2704  CG  PRO B 777      56.561 -10.950  24.291  1.00 56.03           C
ATOM   2705  CD  PRO B 777      57.807 -11.793  24.508  1.00 56.21           C
ATOM   2706  C   PRO B 777      57.189  -9.364  26.737  1.00 54.10           C
ATOM   2707  O   PRO B 777      56.916 -10.338  27.466  1.00 53.82           O
ATOM   2708  N   THR B 778      56.810  -8.103  26.983  1.00 52.28           N
ATOM   2709  CA  THR B 778      55.960  -7.751  28.117  1.00 51.05           C
ATOM   2710  CB  THR B 778      56.128  -6.263  28.526  1.00 51.62           C
ATOM   2711  OG1 THR B 778      57.514  -5.930  28.693  1.00 52.75           O
ATOM   2712  CG2 THR B 778      55.525  -6.018  29.916  1.00 51.07           C
ATOM   2713  C   THR B 778      54.508  -7.973  27.702  1.00 49.65           C
ATOM   2714  O   THR B 778      53.774  -7.020  27.460  1.00 49.64           O
ATOM   2715  N   LEU B 779      54.098  -9.228  27.595  1.00 47.40           N
ATOM   2716  CA  LEU B 779      52.748  -9.548  27.199  1.00 45.15           C
ATOM   2717  CB  LEU B 779      52.486 -11.020  27.483  1.00 44.67           C
ATOM   2718  CG  LEU B 779      53.553 -11.917  26.856  1.00 44.69           C
ATOM   2719  CD1 LEU B 779      53.599 -13.324  27.488  1.00 45.78           C
ATOM   2720  CD2 LEU B 779      53.361 -12.007  25.369  1.00 45.46           C
ATOM   2721  C   LEU B 779      51.739  -8.680  27.941  1.00 44.03           C
ATOM   2722  O   LEU B 779      51.867  -8.480  29.137  1.00 43.69           O
ATOM   2723  N   SER B 780      50.729  -8.184  27.219  1.00 42.70           N
ATOM   2724  CA  SER B 780      49.645  -7.367  27.780  1.00 41.09           C
ATOM   2725  CB  SER B 780      48.967  -6.594  26.642  1.00 41.11           C
ATOM   2726  OG  SER B 780      48.015  -5.655  27.119  1.00 41.62           O
ATOM   2727  C   SER B 780      48.620  -8.238  28.496  1.00 40.22           C
ATOM   2728  O   SER B 780      48.381  -9.353  28.080  1.00 39.24           O
ATOM   2729  N   PRO B 781      47.997  -7.730  29.555  1.00 40.30           N
ATOM   2730  CA  PRO B 781      47.066  -8.528  30.355  1.00 40.49           C
ATOM   2731  CB  PRO B 781      46.795  -7.626  31.569  1.00 40.18           C
ATOM   2732  CG  PRO B 781      46.953  -6.295  31.060  1.00 40.81           C
ATOM   2733  CD  PRO B 781      48.136  -6.369  30.103  1.00 40.81           C
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ATOM   2734  C   PRO B 781      45.775  -8.859  29.620  1.00 40.94           C
ATOM   2735  O   PRO B 781      45.134  -7.961  29.063  1.00 41.63           O
ATOM   2736  N   ILE B 782      45.408 -10.140  29.606  1.00 40.96           N
ATOM   2737  CA  ILE B 782      44.174 -10.590  28.961  1.00 41.15           C
ATOM   2738  CB  ILE B 782      44.169 -12.125  28.886  1.00 41.28           C
ATOM   2739  CG1 ILE B 782      45.321 -12.601  28.000  1.00 41.51           C
ATOM   2740  CD1 ILE B 782      45.027 -12.473  26.509  1.00 42.88           C
ATOM   2741  CG2 ILE B 782      42.817 -12.667  28.388  1.00 40.06           C
ATOM   2742  C   ILE B 782      42.923 -10.093  29.710  1.00 41.48           C
ATOM   2743  O   ILE B 782      42.915  -9.990  30.932  1.00 40.74           O
ATOM   2744  N   PRO B 783      41.877  -9.749  28.967  1.00 41.74           N
ATOM   2745  CA  PRO B 783      40.617  -9.334  29.579  1.00 42.10           C
ATOM   2746  CB  PRO B 783      39.719  -9.080  28.374  1.00 41.64           C
ATOM   2747  CG  PRO B 783      40.666  -8.777  27.311  1.00 41.40           C
ATOM   2748  CD  PRO B 783      41.830  -9.692  27.497  1.00 41.11           C
ATOM   2749  C   PRO B 783      40.049 -10.450  30.413  1.00 43.09           C
ATOM   2750  O   PRO B 783      39.720 -11.490  29.879  1.00 42.35           O
ATOM   2751  N   HIS B 784      39.907 -10.203  31.708  1.00 45.68           N
ATOM   2752  CA  HIS B 784      39.388 -11.196  32.656  1.00 48.44           C
ATOM   2753  CB  HIS B 784      38.831 -10.507  33.902  1.00 49.03           C
ATOM   2754  CG  HIS B 784      38.870 -11.356  35.137  1.00 51.46           C
ATOM   2755  ND1 HIS B 784      38.178 -12.545  35.248  1.00 53.83           N
ATOM   2756  CE1 HIS B 784      38.390 -13.068  36.446  1.00 54.70           C
ATOM   2757  NE2 HIS B 784      39.185 -12.254  37.122  1.00 54.84           N
ATOM   2758  CD2 HIS B 784      39.506 -11.180  36.322  1.00 53.76           C
ATOM   2759  C   HIS B 784      38.331 -12.109  32.048  1.00 49.08           C
ATOM   2760  O   HIS B 784      38.559 -13.299  31.879  1.00 49.44           O
ATOM   2761  N   ILE B 785      37.169 -11.552  31.746  1.00 50.08           N
ATOM   2762  CA  ILE B 785      36.100 -12.296  31.075  1.00 51.26           C
ATOM   2763  CB  ILE B 785      36.409 -12.469  29.563  1.00 51.67           C
ATOM   2764  CG1 ILE B 785      35.162 -12.971  28.831  1.00 52.65           C
ATOM   2765  CD1 ILE B 785      35.332 -13.007  27.347  1.00 54.35           C
ATOM   2766  CG2 ILE B 785      37.583 -13.424  29.341  1.00 50.78           C
ATOM   2767  C   ILE B 785      35.757 -13.651  31.643  1.00 51.63           C
ATOM   2768  O   ILE B 785      35.905 -14.643  30.960  1.00 51.81           O
ATOM   2769  N   PRO B 786      35.313 -13.691  32.890  1.00 52.49           N
ATOM   2770  CA  PRO B 786      34.882 -14.933  33.536  1.00 52.77           C
ATOM   2771  CB  PRO B 786      35.206 -14.656  34.998  1.00 52.72           C
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ATOM   2772  CG  PRO B 786      34.865 -13.198  35.163  1.00 52.87           C
ATOM   2773  CD  PRO B 786      35.236 -12.542  33.817  1.00 53.07           C
ATOM   2774  C   PRO B 786      33.381 -15.174  33.396  1.00 53.40           C
ATOM   2775  O   PRO B 786      32.835 -15.085  32.279  1.00 53.92           O
ATOM   2776  N   ARG B 787      32.730 -15.465  34.527  1.00 53.49           N
ATOM   2777  CA  ARG B 787      31.274 -15.694  34.591  1.00 53.49           C
ATOM   2778  CB  ARG B 787      30.480 -14.416  34.239  1.00 53.44           C
ATOM   2779  CG  ARG B 787      30.063 -13.565  35.449  1.00 52.26           C
ATOM   2780  CD  ARG B 787      31.223 -13.138  36.339  1.00 52.06           C
ATOM   2781  NE  ARG B 787      30.807 -12.649  37.659  1.00 53.17           N
ATOM   2782  CZ  ARG B 787      30.457 -13.428  38.706  1.00 51.86           C
ATOM   2783  NH1 ARG B 787      30.468 -14.750  38.601  1.00 50.85           N
ATOM   2784  NH2 ARG B 787      30.090 -12.880  39.864  1.00 49.91           N
ATOM   2785  C   ARG B 787      30.800 -16.882  33.745  1.00 53.54           C
ATOM   2789  N   LEU P   1      20.931 -14.544  31.252  1.00 47.69           N
ATOM   2790  CA  LEU P   1      22.180 -13.716  31.289  1.00 47.41           C
ATOM   2791  CB  LEU P   1      23.030 -14.044  32.535  1.00 47.97           C
ATOM   2792  CG  LEU P   1      23.458 -15.482  32.878  1.00 48.35           C
ATOM   2793  CD1 LEU P   1      24.423 -15.489  34.063  1.00 49.77           C
ATOM   2794  CD2 LEU P   1      22.266 -16.389  33.165  1.00 48.66           C
ATOM   2795  C   LEU P   1      22.987 -13.883  29.991  1.00 46.60           C
ATOM   2796  O   LEU P   1      22.417 -13.727  28.897  1.00 47.13           O
ATOM   2797  N   ASP P   2      24.287 -14.207  30.109  1.00 44.53           N
ATOM   2798  CA  ASP P   2      25.177 -14.357  28.935  1.00 42.24           C
ATOM   2799  CB  ASP P   2      24.541 -15.300  27.910  1.00 42.69           C
ATOM   2800  CG  ASP P   2      25.522 -15.772  26.866  1.00 44.51           C
ATOM   2801  OD1 ASP P   2      25.766 -15.024  25.896  1.00 45.50           O
ATOM   2802  OD2 ASP P   2      26.093 -16.887  26.932  1.00 46.89           O
ATOM   2803  C   ASP P   2      25.516 -12.983  28.288  1.00 39.49           C
ATOM   2804  O   ASP P   2      26.077 -12.893  27.200  1.00 39.39           O
ATOM   2805  N   TYR P   3      25.145 -11.911  28.970  1.00 35.91           N
ATOM   2806  CA  TYR P   3      25.408 -10.565  28.477  1.00 32.30           C
ATOM   2807  CB  TYR P   3      24.129  -9.724  28.549  1.00 31.47           C
ATOM   2808  CG  TYR P   3      24.334  -8.262  28.269  1.00 31.00           C
ATOM   2809  CD1 TYR P   3      24.418  -7.805  26.965  1.00 29.48           C
ATOM   2810  CE1 TYR P   3      24.583  -6.478  26.693  1.00 27.36           C
ATOM   2811  CZ  TYR P   3      24.676  -5.570  27.712  1.00 27.68           C
ATOM   2812  OH  TYR P   3      24.888  -4.218  27.370  1.00 28.65           O
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ATOM   2813  CE2 TYR P   3      24.582  -5.991  29.034  1.00 25.24           C
ATOM   2814  CD2 TYR P   3      24.407  -7.315  29.309  1.00 27.91           C
ATOM   2815  C   TYR P   3      26.471 -10.014  29.386  1.00 29.47           C
ATOM   2816  O   TYR P   3      26.400 -10.230  30.588  1.00 28.95           O
ATOM   2817  N   HIS P   4      27.456  -9.330  28.820  1.00 26.50           N
ATOM   2818  CA  HIS P   4      28.564  -8.759  29.600  1.00 24.52           C
ATOM   2819  CB  HIS P   4      29.803  -8.571  28.690  1.00 24.64           C
ATOM   2820  CG  HIS P   4      30.980  -7.912  29.349  1.00 25.77           C
ATOM   2821  ND1 HIS P   4      31.453  -8.268  30.598  1.00 30.26           N
ATOM   2822  CE1 HIS P   4      32.496  -7.522  30.917  1.00 27.94           C
ATOM   2823  NE2 HIS P   4      32.732  -6.707  29.910  1.00 26.64           N
ATOM   2824  CD2 HIS P   4      31.790  -6.919  28.926  1.00 27.32           C
ATOM   2825  C   HIS P   4      28.197  -7.412  30.271  1.00 22.87           C
ATOM   2826  O   HIS P   4      28.058  -6.414  29.595  1.00 21.47           O
ATOM   2827  N   PHE P   5      28.025  -7.405  31.590  1.00 21.22           N
ATOM   2828  CA  PHE P   5      27.773  -6.153  32.298  1.00 20.74           C
ATOM   2829  CB  PHE P   5      26.881  -6.357  33.494  1.00 18.47           C
ATOM   2830  CG  PHE P   5      25.501  -6.754  33.152  1.00 16.23           C
ATOM   2831  CD1 PHE P   5      25.193  -8.091  32.917  1.00 14.97           C
ATOM   2832  CE1 PHE P   5      23.887  -8.475  32.631  1.00 13.89           C
ATOM   2833  CZ  PHE P   5      22.881  -7.505  32.578  1.00 11.09           C
ATOM   2834  CE2 PHE P   5      23.182  -6.167  32.806  1.00 10.80           C
ATOM   2835  CD2 PHE P   5      24.471  -5.790  33.087  1.00 11.98           C
ATOM   2836  C   PHE P   5      29.109  -5.609  32.769  1.00 21.26           C
ATOM   2837  O   PHE P   5      29.724  -6.195  33.664  1.00 21.67           O
ATOM   2838  N   GLY P   6      29.556  -4.502  32.170  1.00 21.32           N
ATOM   2839  CA  GLY P   6      30.859  -3.926  32.468  1.00 21.51           C
ATOM   2840  C   GLY P   6      30.831  -2.897  33.585  1.00 22.19           C
ATOM   2841  O   GLY P   6      31.865  -2.528  34.114  1.00 21.62           O
ATOM   2842  N   LEU P   7      29.651  -2.406  33.919  1.00 23.30           N
ATOM   2843  CA  LEU P   7      29.543  -1.497  35.032  1.00 25.46           C
ATOM   2844  CB  LEU P   7      28.154  -0.859  35.099  1.00 25.82           C
ATOM   2845  CG  LEU P   7      27.814   0.211  34.061  1.00 26.11           C
ATOM   2846  CD1 LEU P   7      26.339   0.562  34.191  1.00 24.70           C
ATOM   2847  CD2 LEU P   7      28.709   1.422  34.234  1.00 21.99           C
ATOM   2848  C   LEU P   7      29.817  -2.254  36.323  1.00 26.52           C
ATOM   2849  O   LEU P   7      29.437  -3.421  36.472  1.00 25.30           O
ATOM   2850  N   GLU P   8      30.492  -1.567  37.240  1.00 28.49           N
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ATOM   2851  CA  GLU P   8      30.779  -2.099  38.551  1.00 31.21           C
ATOM   2852  CB  GLU P   8      32.215  -1.763  38.887  1.00 32.54           C
ATOM   2853  CG  GLU P   8      33.179  -2.369  37.881  1.00 38.33           C
ATOM   2854  CD  GLU P   8      34.639  -2.164  38.254  1.00 44.38           C
ATOM   2855  OE1 GLU P   8      34.977  -1.015  38.639  1.00 47.15           O
ATOM   2856  OE2 GLU P   8      35.437  -3.145  38.151  1.00 44.55           O
ATOM   2857  C   GLU P   8      29.830  -1.509  39.593  1.00 30.87           C
ATOM   2858  O   GLU P   8      29.277  -0.443  39.374  1.00 30.40           O
ATOM   2859  N   GLU P   9      29.655  -2.193  40.726  1.00 31.54           N
ATOM   2860  CA  GLU P   9      28.722  -1.742  41.790  1.00 31.59           C
ATOM   2861  CB  GLU P   9      28.841  -2.607  43.057  1.00 32.17           C
ATOM   2862  CG  GLU P   9      28.217  -4.028  42.934  1.00 34.26           C
ATOM   2863  CD  GLU P   9      28.018  -4.747  44.294  1.00 33.72           C
ATOM   2864  OE1 GLU P   9      27.685  -4.084  45.314  1.00 33.47           O
ATOM   2865  OE2 GLU P   9      28.185  -5.978  44.350  1.00 31.42           O
ATOM   2866  C   GLU P   9      28.826  -0.254  42.133  1.00 30.99           C
ATOM   2867  O   GLU P   9      27.826   0.429  42.361  1.00 31.00           O
ATOM   2868  N   GLY P  10      30.033   0.276  42.153  1.00 30.01           N
ATOM   2869  CA  GLY P  10      30.155   1.696  42.418  1.00 29.07           C
ATOM   2870  C   GLY P  10      29.895   2.598  41.209  1.00 27.90           C
ATOM   2871  O   GLY P  10      30.205   3.806  41.240  1.00 28.51           O
ATOM   2872  N   GLU P  11      29.353   2.024  40.138  1.00 25.73           N
ATOM   2873  CA  GLU P  11      29.073   2.791  38.922  1.00 23.64           C
ATOM   2874  CB  GLU P  11      29.952   2.303  37.748  1.00 24.46           C
ATOM   2875  CG  GLU P  11      31.459   2.612  37.875  1.00 26.02           C
ATOM   2876  CD  GLU P  11      32.325   1.859  36.852  1.00 26.65           C
ATOM   2877  OE1 GLU P  11      33.486   2.296  36.631  1.00 24.35           O
ATOM   2878  OE2 GLU P  11      31.853   0.824  36.281  1.00 26.05           O
ATOM   2879  C   GLU P  11      27.603   2.753  38.516  1.00 21.13           C
ATOM   2880  O   GLU P  11      26.905   1.758  38.653  1.00 19.86           O
ATOM   2881  N   GLY P  12      27.131   3.855  38.005  1.00 19.40           N
ATOM   2882  CA  GLY P  12      25.766   3.895  37.535  1.00 18.44           C
ATOM   2883  C   GLY P  12      25.582   4.880  36.401  1.00 17.74           C
ATOM   2884  O   GLY P  12      26.404   5.785  36.161  1.00 16.52           O
ATOM   2885  N   ILE P  13      24.458   4.734  35.719  1.00 17.35           N
ATOM   2886  CA  ILE P  13      24.156   5.570  34.567  1.00 17.40           C
ATOM   2887  CB  ILE P  13      22.680   5.451  34.230  1.00 16.80           C
ATOM   2888  CG1 ILE P  13      22.353   6.275  32.979  1.00 17.71           C
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ATOM   2889  CD1 ILE P  13      23.048   5.763  31.684  1.00 18.51           C
ATOM   2890  CG2 ILE P  13      21.913   5.983  35.380  1.00 17.44           C
ATOM   2891  C   ILE P  13      24.535   7.051  34.805  1.00 17.29           C
ATOM   2892  O   ILE P  13      24.899   7.769  33.896  1.00 17.49           O
ATOM   2893  N   ARG P  14      24.443   7.527  36.022  1.00 16.45           N
ATOM   2894  CA  ARG P  14      24.749   8.917  36.228  1.00 17.18           C
ATOM   2895  CB  ARG P  14      24.232   9.313  37.598  1.00 17.84           C
ATOM   2896  CG  ARG P  14      24.580  10.693  38.068  1.00 17.51           C
ATOM   2897  CD  ARG P  14      25.712  10.655  39.027  1.00 19.60           C
ATOM   2898  NE  ARG P  14      25.496  11.615  40.079  1.00 21.69           N
ATOM   2899  CZ  ARG P  14      26.127  11.610  41.237  1.00 22.46           C
ATOM   2900  NH1 ARG P  14      27.038  10.683  41.515  1.00 20.71           N
ATOM   2901  NH2 ARG P  14      25.840  12.557  42.113  1.00 22.29           N
ATOM   2902  C   ARG P  14      26.228   9.319  36.051  1.00 17.89           C
ATOM   2903  O   ARG P  14      26.533  10.465  35.749  1.00 18.28           O
ATOM   2904  N   ASP P  15      27.153   8.388  36.249  1.00 17.97           N
ATOM   2905  CA  ASP P  15      28.557   8.678  36.058  1.00 17.42           C
ATOM   2906  CB  ASP P  15      29.419   7.620  36.731  1.00 17.17           C
ATOM   2907  CG  ASP P  15      28.943   7.257  38.136  1.00 16.85           C
ATOM   2908  OD1 ASP P  15      28.567   8.168  38.917  1.00 14.72           O
ATOM   2909  OD2 ASP P  15      28.933   6.068  38.549  1.00 17.21           O
ATOM   2910  C   ASP P  15      28.893   8.700  34.576  1.00 18.51           C
ATOM   2911  O   ASP P  15      29.888   9.266  34.154  1.00 19.86           O
ATOM   2912  N   LEU P  16      28.067   8.078  33.752  1.00 19.15           N
ATOM   2913  CA  LEU P  16      28.383   8.009  32.351  1.00 19.27           C
ATOM   2914  CB  LEU P  16      27.482   7.006  31.674  1.00 19.48           C
ATOM   2915  CG  LEU P  16      27.817   5.590  32.121  1.00 18.49           C
ATOM   2916  CD1 LEU P  16      26.903   4.583  31.531  1.00 16.38           C
ATOM   2917  CD2 LEU P  16      29.205   5.334  31.714  1.00 18.61           C
ATOM   2918  C   LEU P  16      28.287   9.373  31.691  1.00 20.34           C
ATOM   2919  O   LEU P  16      28.964   9.619  30.688  1.00 18.95           O
ATOM   2920  N   PHE P  17      27.423  10.216  32.264  1.00 22.07           N
ATOM   2921  CA  PHE P  17      27.160  11.583  31.843  1.00 24.13           C
ATOM   2922  CB  PHE P  17      25.668  11.799  31.553  1.00 23.78           C
ATOM   2923  CG  PHE P  17      25.128  10.936  30.490  1.00 22.61           C
ATOM   2924  CD1 PHE P  17      24.659   9.689  30.789  1.00 21.60           C
ATOM   2925  CE1 PHE P  17      24.142   8.878  29.790  1.00 22.90           C
ATOM   2926  CZ  PHE P  17      24.160   9.321  28.432  1.00 24.90           C
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ATOM   2927  CE2 PHE P  17      24.662  10.542  28.122  1.00 23.17      C
ATOM   2928  CD2 PHE P  17      25.144  11.351  29.158  1.00 24.24      C
ATOM   2929  C   PHE P  17      27.470  12.403  33.045  1.00 26.26      C
ATOM   2930  O   PHE P  17      26.583  13.079  33.582  1.00 26.70      O
ATOM   2931  N   ASP P  18      28.717  12.312  33.505  1.00 29.15      N
ATOM   2932  CA  ASP P  18      29.152  12.999  34.732  1.00 31.05      C
ATOM   2933  CB  ASP P  18      29.110  12.033  35.922  1.00 31.59      C
ATOM   2934  CG  ASP P  18      29.079  12.741  37.254  1.00 35.19      C
ATOM   2935  OD1 ASP P  18      29.132  12.001  38.293  1.00 37.21      O
ATOM   2936  OD2 ASP P  18      29.007  14.012  37.355  1.00 37.60      O
ATOM   2937  C   ASP P  18      30.566  13.540  34.586  1.00 31.76      C
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